Content

- 1. Gromacs topologies with all force field parameters used 2. Coordinates in Gromacs format (*.gro)

Attention: The topologies built with the amb2gmx.pl script. All parameters all from GAFF. The membrane was modeled with the Slipids force field (available for free at http://people.su.se/~jjm, where you also can find coordinates for pre-equilibrated lipid bilayers).

1. Gromacs topologies

1,3,5 trichlorobenzene (gas phase charges)

[moleculetype] ; Name nrexcl 135trichlorobenzene 3										
[atoms; nr ; nr 1 2 3 4 5 6 7 8 9 10 11 12] type ca ha ca ca ca ha ca ca ha ca ca ha ca ca ca ca ca ca ca ca ca ca ca ca ca	resnr re 1 1 1 1 1 1 1 1 1 1 1 1 1 1	esidue at LIG LIG LIG LIG LIG LIG LIG LIG LIG LIG	om cg C1 H2 C3 C4 H5 C6 C7 H8 C9 L1 L2 L3	nr 1 2 3 5 6 7 7 8 9 - 7 10 - 11 - 12 -	charge 0.1646 0.2043 0.1646 0.1044 0.2043 0.1646 0.1044 0.2043 0.1044 0.2043 0.0647 0.0647	$\begin{array}{c} \text{mass} \\ 12.00000 \\ 1.00000 \\ 12.00000 \\ 12.00000 \\ 1.00000 \\ 12.00000 \\ 12.00000 \\ 12.00000 \\ 35.50000 \\ 35.50000 \\ 35.50000 \\ 35.50000 \end{array}$	typeB	chargeB	
<pre>[bonds ; ai 1 4 7 1 1 3 3 4 6 7 9</pre>] aj funct 2 1 5 1 8 1 3 1 9 1 4 1 12 1 6 1 7 1 11 1 9 1 10 1	r k 1.0870e- 1.0870e- 1.3870e- 1.3870e- 1.3870e- 1.3870e- 1.3870e- 1.7290e- 1.3870e- 1.7290e-	01 2.881 01 2.881 01 2.881 01 4.003 01 4.003 01 2.701 01 4.003 01 4.003 01 4.003 01 4.003 01 2.701 01 2.701 01 2.701 01 2.701	1e+05 1e+05 3e+05 3e+05 3e+05 3e+05 3e+05 3e+05 3e+05 3e+05 2e+05 3e+05 2e+05						
<pre>[pairs ; ai 1 1 2 2 2 2 4 5 5 5 8 8 1 3 3 9 6 6 9 9</pre>] aj funct 5 8 4 12 7 10 8 12 7 11 11 10 6 7 10 11 11 4 12 10 12 11	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1								
[angles; ai ; ai 2 3 5 6 8 1 1 1 1 3 4 4 4 6 7 7	$\begin{bmatrix} s \\ a \\ j \\ a \\ 1 \\ 3 \\ 1 \\ 3 \\ 1 \\ 9 \\ 4 \\ 5 \\ 4 \\ 6 \\ 7 \\ 9 \\ 3 \\ 4 \\ 3 \\ 12 \\ 9 \\ 7 \\ 9 \\ 10 \\ 1 \\ 9 \\ 10 \\ 1 \\ 9 \\ 6 \\ 11 \\ 9 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 $	funct th 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	teta cth 2001e+02 2001e+02 2001e+02 2001e+02 2001e+02 1940e+02 1997e+02 1997e+02 1997e+02 1997e+02 1997e+02 1997e+02 19940e+02 1997e+02 19940e+02	$\begin{array}{c} 4.0551\\ 4.0551\\ 4.0551\\ 4.0551\\ 4.0551\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ 5.2651\\ \end{array}$	e+02 e+02 e+02 e+02 e+02 e+02 e+02 e+02					
[dihedn ;i j 1 1	rals] k 1 3 4 9 7	func C 5 3 8 3	0 C5 3 30.334 3 30.334	100 100	0.0000	00 -30 00 -30	.33400 .33400	0.00000 0.00000	0.00000 0.00000	

0.00000 ; 0.00000 ;

2	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	3	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	
2	1	9	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	
2	1	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	:
4	6	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	:
5	4	3	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	:
5	4	6	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	4	6	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	7	6	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	7	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	9	3	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	6	4	5	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
6	9	7	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	3	4	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	9	7	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	1	9	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	1	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	6	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	4	6	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	6	7	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	4	3	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	7	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	3	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	7	6	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	4	3	12	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
4	7	6	11	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	7	9	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
end											

1,3,5 trichlorobenzene (polarized charges, water)

[moleculetype] ; Name nrexcl 135trichlorobenzene 3

100 ti i chi toi obenzene	5
[atoms]	

							-		_
chargeB	mass typeB	charge	cgnr	atom	residue	resnr	type	nr	;
•	12.000000	0.16220	1	C1	LIG	1	ca	1	
	1.000000	0.11750	2	H2	LIG	1	ha	2	
	12.000000	-0.20170	3	C3	LIG	1	ca	3	
	12.000000	0.16220	4	C4	LIG	1	ca	4	
	1.000000	0.11750	5	H5	LIG	1	ha	5	
	12.000000	-0.20170	6	C6	LIG	1	ca	6	
	12.000000	0.16220	7	C7	LIG	1	ca	7	
	1.000000	0.11750	8	H8	LIG	1	ha	8	
	12.000000	-0.20170	9	C9	LIG	1	ca	9	
	35.500000	-0.07800	10	CL1	LIG	1	cl	10	
	35.500000	-0.07800	11	CL2	LIG	1	cl	11	
	35.500000	-0.07800	12	CL3	LIG	1	cl	12	

[bonds]

;	ai	aj	funct	r k	
	1	Ž	1	1.0870e-01	2.8811e+05
	4	5	1	1.0870e-01	2.8811e+05
	7	8	1	1.0870e-01	2.8811e+05
	1	3	1	1.3870e-01	4.0033e+05
	1	9	1	1.3870e-01	4.0033e+05
	3	4	1	1.3870e-01	4.0033e+05
	3	12	1	1.7290e-01	2.7012e+05
	4	6	1	1.3870e-01	4.0033e+05
	6	7	1	1.3870e-01	4.0033e+05
	6	11	1	1.7290e-01	2.7012e+05
	7	9	1	1.3870e-01	4.0033e+05
	9	10	1	1.7290e-01	2.7012e+05

7 9

Ε	pairs]	
;	ai	aj funct	
	1	້ 5	1
	1	8	1
	2	4	1
	2	12	1
	2	7	1
	2	10	1
	4	8	1
	5	12	1
	5	7	1
	5	11	1
	8	11	1
	8	10	1
	1	6	1
	3	7	1
	3	10	1
	3	11	1
	9	4	1
	6	12	1
	6	10	1
	9	12	1
	9	11	1

6 7 9 1 1.1997e+02 5.6216e+02 7 6 11 1 1.1940e+02 5.2651e+02 7 9 10 1 1.1940e+02 5.2651e+02							51e+02 51e+02 51e+02 51e+02 51e+02 51e+02 51e+02 51e+02 16e+02 51	4.055 4.055 4.0555 5.626 5.6262 5.6262 5.62626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.626262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.6266262 5.626626262 5.626626262 5.62662626262 5.6266262626262 5.62662626262626262626262626262626262626	a cth D1e+02 D1e+02 D1e+02 D1e+02 D1e+02 D1e+02 D7e+02 40e+02 D7e+02 40e+02 D7e+02 40e+02 D7e+02 40e+02 40e+02 40e+02 40e+02 40e+02	thet 1.20 1.20 1.20 1.20 1.19 1.19 1.19 1.19 1.19 1.19 1.19 1.1	funct 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	ak 3 9 5 6 8 9 4 12 7 10 9 6 12 7 11 9 11] j a 1 4 4 7 7 3 3 9 9 1 4 3 6 6 7 6 9	angles ai 2 3 5 6 8 1 1 1 3 3 4 4 4 6 7 7	Ε;
$ \begin{bmatrix} dihedrals \end{bmatrix} \\ \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	 0.000000	0000 0000 0000 0000 0000 0000 0000 0000 0000	$egin{array}{cccc} 0.0000\\ 0.000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.$	00000 00000 00000 00000 00000 00000 0000	30.33400 30.30000000000	00 00 00 00 00 00 00 00 00 00 00 00 00	0.000 0.000	400 400 400 400 400 400 400 400 400 400	CE 30.33 3	000000000000000000000000000000000000000	func 5 8 4 12 7 10 8 12 7 11 10 8 12 7 11 10 3 5 8 6 6 7 10 12 11 10 12 7 11 10 10 10 10 11 10 10 10 10	473399736669947479966373936369	als] k 1 9 1111164447771693911144166477177477	dihedr j 1 1 2 2 2 2 4 5 5 8 8 2 3 6 1 1 3 3 3 9 4 6 6 9 9 1 4 1 2 2 2 2 4 5 5 5 8 8 2 3 6 1 1 3 3 3 9 4 6 6 9 9 1 4 1 2 2 2 2 2 2 4 5 5 5 8 8 8 2 3 6 1 1 3 3 3 9 4 6 6 9 9 1 4 1 2 2 2 2 2 4 5 5 5 8 8 8 2 3 6 1 1 3 3 3 9 4 6 6 9 9 1 4 1 2 2 2 2 2 4 5 5 5 8 8 8 2 3 6 1 1 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 3 3 3 3 9 4 6 6 9 9 1 4 1 4 1 1 1 1 1 1 1 1 1 1 1 1 1	[;i

1,3,5 trichlorobenzene (polarized charges, hexadecane)

typeB

chargeB

E	molecu	ulety	pe]						
;	Name			nrexcl					
С	1X		3						
E	atoms]							
;	nr		type	resnr	residue	atom	cgnr	charge	mass
	1		ca	1	LI	G C1	1	0.1634	12.000000
	2		ha	1	LI	G H2	2	0.1099	1.000000
	3		ca	1	LI	G C3	3	-0.2028	12.000000
	4		ca	1	LI	G C4	4	0.1634	12.000000
	5		ha	1	LI	G H5	5	0.1099	1.000000
	6		ca	1	LI	G C6	6	-0.2028	12.000000
	7		ca	1	LI	G C7	7	0.1634	12.000000
	8		ha	1	LI	G H8	8	0.1099	1.000000
	9		ca	1	LI	G C9	9	-0.2028	12.000000
	10		cl	1	LI	G CL1	10	-0.0705	35.500000
	11		cl	1	LI	G CL2	11	-0.0705	35.500000
	12		cl	1	LI	G CL3	12	-0.0705	35.500000
г	bonds	1							
:	ai		funct	r k					
,	1	~j.	1	1 0870	a = 01 2	88110+0	5		
	Å	5	1	1 0870	a = 01 2	88110+0	5		

	~ ~		1.00100 01	2.00110.00
4	5	1	1.0870e-01	2.8811e+05
7	8	1	1.0870e-01	2.8811e+05
1	3	1	1.3870e-01	4.0033e+05
1	9	1	1.3870e-01	4.0033e+05
3	4	1	1.3870e-01	4.0033e+05
3	12	1	1.7290e-01	2.7012e+05
4	6	1	1.3870e-01	4.0033e+05
6	7	1	1.3870e-01	4.0033e+05
6	11	1	1.7290e-01	2.7012e+05
7	9	1	1.3870e-01	4.0033e+05
9	10	1	1.7290e-01	2.7012e+05



Chlorobenzene (gas phase charges)

[moleculetype] ; Name Chlorobenzene	nrexcl 3			
[atoms] ; nr type 1 ca 2 ha 3 ca 4 ha 5 ca 6 ha 7 ca 8 ha 9 ca 10 ha 11 ca 12 cl	$\begin{array}{cccccccc} {\rm resnr\ residue} & {\rm atom} & c_{\rm f} \\ 1 & {\rm LIG} & {\rm C} \\ 1 & {\rm LIG} & {\rm H} \\ 1 & {\rm LIG} & {\rm C1} \\ 1 & {\rm LIG} & {\rm C1} \\ 1 & {\rm LIG} & {\rm H1} \\ 1 & {\rm LIG} & {\rm H2} \\ 1 & {\rm LIG} & {\rm H2} \\ 1 & {\rm LIG} & {\rm H3} \\ 1 & {\rm LIG} & {\rm C3} \\ 1 & {\rm LIG} & {\rm C4} \\ 1 & {\rm LIG} & {\rm H4} \\ 1 & {\rm LIG} & {\rm C5} \\ 1 & {\rm LIG} & {\rm CL} \\ \end{array}$	gnr charge mass 1 -0.0781 12.000000 2 0.1266 1.000000 4 0.1454 1.000000 5 -0.1519 12.000000 6 0.1464 1.000000 7 -0.1519 12.000000 8 0.1464 1.000000 9 -0.0781 12.000000 10 0.1266 1.000000 11 0.0489 12.000000 12 -0.1300 35.500000	typeB chargeB	
$\begin{bmatrix} bonds \\ ; ai \\ 1 \\ 2 \\ 1 \\ 3 \\ 4 \\ 1 \\ 5 \\ 6 \\ 1 \\ 7 \\ 8 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	r k 1.0870e-01 2.8811e+05 1.0870e-01 2.8811e+05 1.0870e-01 2.8811e+05 1.0870e-01 2.8811e+05 1.0870e-01 2.8811e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.7290e-01 2.7012e+05			
$ \begin{bmatrix} pairs \\ ai \\ aj funct \\ 1 \\ 0 \\ 2 \\ 4 \\ 2 \\ 5 \\ 2 \\ 9 \\ 2 \\ 12 \\ 3 \\ 8 \\ 11 \\ 4 \\ 6 \\ 4 \\ 7 \\ 5 \\ 10 \\ 6 \\ 8 \\ 11 \\ 4 \\ 6 \\ 4 \\ 7 \\ 5 \\ 10 \\ 8 \\ 11 \\ 10 \\ 12 \\ 1 \\ 7 \\ 3 \\ 9 \\ 3 \\ 12 \\ 11 \\ 5 \\ 7 \\ 12 $	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1			
$\begin{bmatrix} angles \\ i \\ ai \\ 1 \\ 3 \\ 2 \\ 1 \\ 3 \\ 2 \\ 1 \\ 1 \\ 3 \\ 5 \\ 6 \\ 4 \\ 3 \\ 5 \\ 5 \\ 7 \\ 8 \\ 6 \\ 5 \\ 7 \\ 7 \\ 9 \\ 10 \\ 9 \\ 11 \\ 1 \\ 3 \\ 5 \\ 1 \\ 11 \\ 9 \\ 1 \\ 11 \\ 12 \\ 3 \\ 5 \\ 7 \\ 5 \\ 7 \\ 9 \\ 10 \\ 9 \\ 11 \\ 11 \\ 12 \\ 3 \\ 1 \\ 11 \\ 12 \\ 3 \\ 1 \\ 11 \\ 1$	funct theta cth 1 1.2001e+02 4.055 1 1.2001e+02 5.6210 1 1.1997e+02 5.6210 1 1.1940e+02 5.2650	1e+02 1e+02 1e+02 1e+02 1e+02 1e+02 1e+02 1e+02 1e+02 1e+02 6e+02 6e+02 6e+02 6e+02 6e+02 6e+02 6e+02 1e+02		
$\begin{bmatrix} dihedrals \\ j & k \\ 1 & 3 & 5 \\ 1 & 11 & 9 \\ 2 & 1 & 3 \\ 2 & 1 & 3 \\ 2 & 1 & 1 \\ 2 & 1 & 11 \\ 2 & 1 & 11 \\ 3 & 5 & 7 \\ 11 & 1 & 3 \end{bmatrix}$	$\begin{array}{cccccccc} {\rm func} & {\rm C0} & \dots & {\rm C5} \\ 6 & 3 & 30.33400 \\ 10 & 3 & 30.33400 \\ 4 & 3 & 30.33400 \\ 5 & 3 & 30.33400 \\ 9 & 3 & 30.33400 \\ 12 & 3 & 30.33400 \\ 8 & 3 & 30.33400 \\ 4 & 3 & 30.33400 \end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	0.00000 0.0000 0.00000 0.0000 0.00000 0.0000 0.00000 0.0000 0.00000 0.0000 0.00000 0.0000 0.00000 0.0000 0.00000 0.0000	00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ; 00 0.00000 ;

4 5 6 8 8 10 2 1 3 5 7 1 1 3 3 3 11 5 7 1 end	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 6 \\ 7 \\ 10 \\ 8 \\ 9 \\ 10 \\ 11 \\ 1 \\ 1 \\ 4 \\ 6 \\ 8 \\ 10 \\ 7 \\ 7 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	$\begin{array}{c} 30.33400\\ 30.33400\\ 30.33400\\ 30.33400\\ 30.33400\\ 30.33400\\ 30.33400\\ 9.20480\\ 9.20480\\ 9.20480\\ 9.20480\\ 9.20480\\ 30.33400\\ 30.3$		0000 -33 0000 -30 0000 -33 0000 -33 0000 -33 0000 -33 0000 -33 0000 -33 0000 -33 0000 -43 0000 -43 0000 -33 0000 -33 0000 -33 0000 -33 0000 -33 0000 -33 0000 -33 0000 -34 0000 -33 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 0000 -34 <th>0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.20480 0.20480 0.20480 0.33400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 00</th> <th>0.00000 0.00000</th> <th>$egin{array}{cccc} 0.00000\\ 0.0000\\$</th> <th>0.00000 0.00000</th> <th>, , , , , , , , , , , , , , , , , , ,</th>	0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.33400 0.20480 0.20480 0.20480 0.33400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 0.3400 00	0.00000 0.00000	$egin{array}{cccc} 0.00000\\ 0.0000\\$	0.00000 0.00000	, , , , , , , , , , , , , , , , , , ,
[molecu	Chlorobenzene (polarized charges, water)										
; Name Chlorobe	; Name nrexcl Chlorobenzene 3										
L atoms ; nr 1 2 3 4 5 6 7 8 9 10 11 11	J tyj	pe res ca ha ca ha ca ha ca ha ca ha ca ca ca	nr resid 1 L1 1 L1	ue atom IG C IG H1 IG C2 IG H2 IG H2 IG C3 IG H3 IG C4 IG C4 IG C4 IG C4 IG C4 IG C5 IG C4	cgnr 1 2 3 4 5 6 7 8 9 10 11 12	charge -0.09190 0.14220 0.16130 0.16390 -0.16260 0.16490 0.16470 -0.09190 0.14220 0.04540 -0.15300	mass 12.00000 1.00000 12.00000 12.00000 12.00000 12.00000 12.00000 12.00000 12.00000 12.00000 12.00000 35.500000	typeB	chargeB		
[bonds ; ai 3 5 7 9 1 1 3 5 7 9 11] aj fund 2 4 6 8 10 3 11 5 7 9 11 12	ct r 1 1.0 1 1.0 1 1.0 1 1.0 1 1.0 1 1.3 1 1.5 1 1	k 870e-01 870e-01 870e-01 870e-01 870e-01 870e-01 870e-01 870e-01 870e-01 870e-01 290e-01	2.8811e+0 2.8811e+0 2.8811e+0 2.8811e+0 2.8811e+0 4.0033e+0 4.0033e+0 4.0033e+0 4.0033e+0 2.7012e+0	5 5 5 5 5 5 5 5 5 5 5 5 5						
<pre>[pairs ; ai 1 1 2 2 2 2 3 11 4 4 5 6 6 8 8 10 1 3 3 11 7</pre>] aj fum 6 10 4 5 9 12 8 4 6 7 10 8 9 10 11 12 7 9 12 5 12	ct 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1									
[angles; ai ; ai 2 2 3	angles] ai aj ak funct theta cth 1 3 4 1 1.2001e+02 4.0551e+02 2 1 3 1 1.2001e+02 4.0551e+02 2 1 11 1 1.2001e+02 4.0551e+02 3 5 6 1 1.2001e+02 4.0551e+02										

4 5 6 7 8 10 1 1 3 5 7 9	3 7 9 7 9 3 11 11 5 7 9 11	5 8 7 10 9 11 5 9 12 11 7 9 11 12	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1.20 1.20 1.20 1.20 1.20 1.19 1.19 1.19 1.19 1.19 1.19 1.19 1.1	001e+02 4.055 001e+02 5.621 997e+02 5.265	1e+02 1e+02 1e+02 1e+02 1e+02 1e+02 6e+02 6e+02 6e+02 6e+02 6e+02 6e+02 6e+02 6e+02 1e+02						
[dihed	rals 1											
;i j	k l		func	CO	C5							
, 1 1	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
1	11	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
2	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
2	1	3 11	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
2	1	11	9 12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	,	
3	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	,	
11	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
4	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
4	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
5	7	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
6	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
6	5	(9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
0	7	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
10	à	9 11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000		
2	1	11	3	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
1	5	3	4	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
3	7	5	6	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
5	9	7	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
7	11	9	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
1	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
1	11	9	1	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
3	1	11	9 12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	,	
3	5	7	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
11	ĭ	3	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
5	7	9	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
7	9	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
1	9	11	12	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
end												

Chlorobenzene (polarized charges, hexadecane)

[moleculetype] ; Name Chlorobenzene nrexcl 3

[atoms]									
; nr	type	resnr	residue	atom	cgnr	charge	mass	typeB	chargeB
1	ca	1	LIG	С	Ŭ 1	-0.0836	12.000000		0
2	ha	1	LIG	Н	2	0.1326	1.000000		
3	ca	1	LIG	C1	3	-0.1542	12.000000		
4	ha	1	LIG	H1	4	0.1521	1.000000		
5	ca	1	LIG	C2	5	-0.1556	12.000000		
6	ha	1	LIG	H2	6	0.1531	1.000000		
7	ca	1	LIG	C3	7	-0.1556	12.000000		
8	ha	1	LIG	H3	8	0.1531	1.000000		
9	ca	1	LIG	C4	9	-0.0836	12.000000		
10	ha	1	LIG	H4	10	0.1326	1.000000		
11	ca	1	LIG	C5	11	0.0499	12.000000		
12	cl	1	LIG	CL	12	-0.1408	35.500000		

[bonds ; ai 3 5 7 9 1 1 3] aj fund 2 4 6 8 10 3 11 5	t 1 1 1 1 1 1 1 1	r k 1.0870e-01 1.0870e-01 1.0870e-01 1.0870e-01 1.0870e-01 1.3870e-01 1.3870e-01	2.8811e+05 2.8811e+05 2.8811e+05 2.8811e+05 2.8811e+05 4.0033e+05 4.0033e+05 4.0033e+05
9	11	1	1.3870e-01	4.0033e+05
11	12	T	1.7290e-01	2.7012e+05
[pairs]			
; ai	aj func	t		
1	6		1	
1	10		1	
2	4		T	

$\begin{array}{cccccccccccccccccccccccccccccccccccc$			
$\left[\begin{array}{cccccccccccccccccccccccccccccccccccc$	theta cth 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.2001e+02 4.0551e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.1997e+02 5.6216e+02 1.19940e+02 5.2651e+02		
$ \begin{bmatrix} dihedrals \\ j & k & 1 & func \\ 1 & 3 & 5 & 6 \\ 1 & 111 & 9 & 10 \\ 2 & 1 & 3 & 4 \\ 2 & 1 & 3 & 5 \\ 2 & 1 & 11 & 9 \\ 2 & 1 & 11 & 12 \\ 3 & 5 & 7 & 8 \\ 111 & 1 & 3 & 4 \\ 4 & 3 & 5 & 6 \\ 4 & 3 & 5 & 7 \\ 5 & 7 & 9 & 10 \\ 6 & 5 & 7 & 8 \\ 6 & 5 & 7 & 9 & 10 \\ 6 & 5 & 7 & 9 & 10 \\ 6 & 5 & 7 & 9 & 10 \\ 6 & 5 & 7 & 9 & 10 \\ 6 & 5 & 7 & 9 & 10 \\ 8 & 7 & 9 & 10 \\ 1 & 3 & 5 & 6 \\ 5 & 9 & 7 & 8 \\ 7 & 11 & 9 & 10 \\ 1 & 3 & 5 & 7 \\ 1 & 11 & 9 & 7 \\ 3 & 1 & 11 & 9 \\ 1 & 1 & 3 & 5 \\ 5 & 7 & 9 & 11 \\ 1 & 1 & 3 & 5 \\ 5 & 7 & 9 & 11 \\ 1 & 1 & 3 & 5 \\ 5 & 7 & 9 & 11 \\ 7 & 9 & 11 & 12 \\ 1 & 9 & 11 & 12 \\ 1 & 9 & 11 & 12 \\ \end{bmatrix} $	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.00000 0.00000 ; 0.00000 0.00000 ; <td< td=""></td<>

end------

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics This journal is $\ensuremath{\mathbb{C}}$ The Owner Societies 2013

Chloroform (gas phase charges)

[moleculet; ; Name C1X	ype] 3	rexcl	
[atoms] ; nr 1 2 3 4 5	type c3 h3 c1 c1 c1	resnr residue atom cgnr charge mass typeB chargeB 1 LIG C 1 -0.5151 12.000000 1 LIG H 2 0.3303 1.000000 1 LIG CL 3 0.0616 35.500000 1 LIG Cl1 4 0.0616 35.500000 1 LIG Cl2 5 0.0616 35.500000	
[bonds] ; ai aj 1 2 1 3 1 4 1 5	funct 1 1 1	r k 1.0950e-01 2.7899e+05 1.7860e-01 2.3347e+05 1.7860e-01 2.3347e+05 1.7860e-01 2.3347e+05	
[pairs] ; ai aj	funct		
[angles] ; ai aj 2 1 2 1 2 1 3 1 3 1 4 1	ak 3 4 5 4 5 5	unct theta cth 1 1.0765e+02 3.6284e+02 1 1.0765e+02 3.6284e+02 1 1.0765e+02 3.6284e+02 1 1.1103e+02 5.2467e+02 1 1.1103e+02 5.2467e+02 1 1.1103e+02 5.2467e+02	
end			
[moleculet; ; Name Chloroform	ype]	rexcl 3	
[atoms] ; nr 1 2 3 4 5	type c3 h3 c1 c1 c1	resnr residue atom cgnr charge mass typeB chargeB 1 LIG C 1 -0.5699 12.000000 1 LIG H 2 0.3935 1.000000 1 LIG CL 3 0.0588 35.500000 1 LIG Cl1 4 0.0588 35.500000 1 LIG Cl2 5 0.0588 35.500000	
[bonds] ; ai aj 1 2 1 3 1 4 1 5	funct 1 1 1	r k 1.0950e-01 2.7899e+05 1.7860e-01 2.3347e+05 1.7860e-01 2.3347e+05 1.7860e-01 2.3347e+05	
[pairs] ; ai aj	funct		
[angles] ; ai aj 2 1 2 1 3 1 3 1 4 1	ak 3 4 5 4 5 5	unct theta cth 1 1.0765e+02 3.6284e+02 1 1.0765e+02 3.6284e+02 1 1.0765e+02 3.6284e+02 1 1.103e+02 5.2467e+02 1 1.1103e+02 5.2467e+02 1 1.1103e+02 5.2467e+02	
end		Chloroform (polarized charges, hexadecane)	
[moleculet; ; Name Chloroform	ype]	rexcl 3	
[atoms] ; nr 1 2 3 4 5	type c3 h3 c1 c1 c1	resnr residue atom cgnr charge mass typeB chargeB 1 LIG C 1 -0.5308 12.000000 1 LIG H 2 0.3508 1.000000 1 LIG CL 3 0.6600 35.500000 1 LIG Cl1 4 0.0600 35.500000 1 LIG Cl2 5 0.0600 35.500000	
[bonds] ; ai aj 1 2 1 3 1 4 1 5	funct 1 1 1	r k 1.0950e-01 2.7899e+05 1.7860e-01 2.3347e+05 1.7860e-01 2.3347e+05 1.7860e-01 2.3347e+05	

[F	bairs]					
; 1	ai	aj	funct				
[a	angles	;]					
;	aĭ	aj	ak f	unct	theta cth		
	2	ĭ	3	1	1.0765e+02	3.6284e+02	
	2	1	4	1	1.0765e+02	3.6284e+02	
	2	1	5	1	1.0765e+02	3.6284e+02	
	3	1	4	1	1.1103e+02	5.2467e+02	
	3	1	5	1	1.1103e+02	5.2467e+02	
	4	1	5	1	1.1103e+02	5.2467e+02	
end	1						

2,4,5 trichloroaniline (gas phase charges)

[molec ; Name 245tric	uletype] hloroanilir	nrexcl ne 3	
[atoms ; nr 1 2 3 4 5 6 6 7 7 8 9 10 11 12 13 14] type ca ca ca ca ca ca ca ca ca ca ca ca ca	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
[bonds ; ai 2 6 12 12 1 1 1 2 4 4 5 5 6 8] aj funct 3 1 7 1 13 1 14 1 2 1 8 1 9 1 4 1 5 1 11 1 12 1 8 1 12 1 8 1 10 1	r k 1.0870e-01 2.8811e+05 1.0870e-01 2.8811e+05 1.0140e-01 3.3572e+05 1.0140e-01 3.3572e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05 1.3840e-01 3.7572e+05 1.3870e-01 4.0033e+05 1.3870e-01 4.0033e+05	
<pre>[pairs ; ai</pre>] aj funct 7 3 5 11 7 13 14 13 14 12 10 5 11 6 10 12 4 4 4 10 11 6 12 10 11 12 10 12	1 1 1 1 1 1 1 1 1 1 1 1 1 1	
[angle ; 1 3 5 5 7 13 1 1 1 2 2 2 2 4 4 5 5 6 6 8	$ \begin{array}{c} s \\ a_{j} \\ 2 \\ 3 \\ 2 \\ 4 \\ 6 \\ 7 \\ 12 \\ 13 \\ 12 \\ 14 \\ 6 \\ 8 \\ 12 \\ 14 \\ 2 \\ 4 \\ 8 \\ 6 \\ 8 \\ 10 \\ 1 \\ 8 \\ 1 \\ 9 \\ 4 \\ 11 \\ 5 \\ 6 \\ 5 \\ 12 \\ 4 \\ 11 \\ 5 \\ 6 \\ 5 \\ 12 \\ 4 \\ 11 \\ 5 \\ 6 \\ 5 \\ 12 \\ 8 \\ 10 \\ 1 \\ 9 \\ 4 \\ 11 \\ 5 \\ 6 \\ 5 \\ 12 \\ 8 \\ 10 \\ 1 \\ 9 \\ 1 \\ 9 \\ 1 \\ 9 \\ 1 \\ 9 \\ 1 \\ 9 \\ 1 \\ 9 \\ 1 \\ 9 \\ 1 \\ 1$	<pre>funct theta cth 1 1.2001e+02 4.0551e+02 1 1.2001e+02 4.0551e+02 1 1.2001e+02 4.0551e+02 1 1.2001e+02 4.0551e+02 1 1.1613e+02 4.1070e+02 1 1.1613e+02 4.1070e+02 1 1.2001e+02 4.0551e+02 1 1.1485e+02 3.3514e+02 1 1.1997e+02 5.6216e+02 1 1.1997e+02 5.6216e+02 1 1.1997e+02 5.2651e+02 1 1.1940e+02 5.2651e+02 1 1.1940e+02 5.2651e+02 1 1.1997e+02 5.6216e+02 1 1.1940e+02 5.2651e+02 1 1.1940e+02 5.2651e+02 1 1.1940e+02 5.6216e+02 1 1.1940e+02 5.6216e+02 1 1.1940e+02 5.6216e+02 1 1.1940e+02 5.6251e+02 1 1.1940e+02 5.6251e+02 </pre>	

[dihed	lrals]										
;i j	k l		func	CO	C5						
ĭ	8	6	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	2	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	2	4	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	12	13	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
4	5	12	14	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	
6	5	12	13	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
6	5	12	14	3	8.78640	0.00000	-8.78640	0.00000	0.00000	0.00000	;
7	6	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	6	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	4	2	3	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
5	8	6	7	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
5	13	12	14	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	
1	2	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	4	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	8	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	8	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	4	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	4	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	1	2	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	2	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	6	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	4	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	8	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	6	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
11	4	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	8	2	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
2	5	4	11	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
4	6	5	12	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	6	8	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;

end----- 2,4,5 trichloroaniline (polarized charges, water)

[; C1	moleculet Name X	ype] 3	nrexcl						
Γ;	atoms] nr 1 2 3 4 5 6 7 8 9 10 11 12 13 14	type ca ca ca ca ca ca ca cl cl cl nh hn hn	resnr resid 1 L 1 L 1 L 1 L 1 L 1 L 1 L 1 L	iue atom IG C IG C1 IG H IG C2 IG C3 IG C4 IG C5 IG C12 IG C12 IG N IG H2 IG H3	cgnr 1 2 3 4 5 6 7 8 9 10 11 12 13 14	charge -0.13550 0.09760 0.14930 -0.31550 0.73590 -0.43780 0.22190 0.14170 -0.10130 -0.09310 -0.08520 -1.16050 0.49130	mass 12.00000 12.00000 12.00000 12.00000 12.00000 12.00000 12.00000 35.50000 35.50000 35.50000 14.00000 1.00000 1.00000	typeB	chargeB
Γ;	bonds] ai aj 2 3 6 7 12 13 12 14 1 2 1 8 1 9 2 4 4 5 4 11 5 6 5 12 6 8 8 10	funct 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	r k 1.0870e-01 1.0140e-01 1.0140e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.3870e-01 1.7290e-01	2.8811e+(2.8811e+(3.3572e+(4.0033e+(4.0033e+(4.0033e+(4.0033e+(2.7012e+(4.0033e+(3.7572e+(4.0033e+(2.7012e+(2.7012e+(05 05 05 05 05 05 05 05 05 05 05 05 05 0				
[;	pairs] ai aj 1 8 9 3 3 4 4 4 4	funct 7 3 5 11 7 13	1 1 1 1 1 1 1						

Electronic Supplementary Material	(ESI) for Physical	Chemistry Chemical	Physics
This journal is © The Owner Societ	ies 2013		

1

1 1 1

1

10

12

end-----

11

<pre>[ang] ; ai 1 3 5 5 5 7 7 13 1 1 1 1 2 2 2 2 2 4 4 5 5 6 6 8</pre>	Les] aj 2 6 12 12 6 12 12 6 12 12 6 12 2 8 8 1 1 4 4 5 5 4 6 5 8 1	ak 3 4 7 13 14 8 14 4 6 10 8 9 9 5 5 11 11 6 6 122 11 11 18 8 22 10 9	funct 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	thet 1.20 1.20 1.16 1.16 1.19 1.19 1.19 1.19 1.19 1.20 1.19 1.20 1.19 1.20 1.19 1.20 1.19	a cth 01e+02 4.05 01e+02 4.05 01e+02 4.05 13e+02 4.10 01e+02 4.05 85e+02 3.35 97e+02 5.62 97e+02 5.62 97e+02 5.62 97e+02 5.62 97e+02 5.62 13e+02 5.80 40e+02 5.62 13e+02 5.80 40e+02 5.26 97e+02 5.62 13e+02 5.80 40e+02 5.26 97e+02 5.62 13e+02 5.80 40e+02 5.26 13e+02 5.80 14e+02 5.26 14e+02 5.26 14e+02 5.26 14e+02 5.26 14e+02 5.26 14e+02 5.26 14e+02 5.26 14e+02 5.26	51e+02 51e+02 70e+02 70e+02 51e+02 14e+02 16e+02 51e+02 16e+02 51e+02 16e+02 51e+02 16e+02 24e+02 51e+02 16e+02 24e+02 51e+02				
[dihe ; i j 3 3 4 4 4 6 6 7 7 1 5 5 1 1 1 2 2 2 8 9 4 5 5 9 8 9 1 1 9 2	drals 1 k 1 1 2 2 5 5 5 5 6 6 4 8 1 1 2 2 2 5 5 5 5 5 6 6 4 8 1 1 4 1 1 5 6 5 1 6 6 4 8 1 4 1 1 5 6 5 1 6 6 4 8 1 2 2 8 1 1 4 4 1 1 5 6 5 1 6 1 1 4 1 1 5 6 5 1 6 1 4 1 5 1 5 1 6 1 4 1 5 1 5 1 6 1 4 1 5 1 5 1 6 1 4 1 5 1 5 1 6 1 4 1 5 1 6 1 6 1 7 1 6 1 7	$\begin{bmatrix} 6 & 2 & 2 & 4 & 4 & 6 & 122 & 122 & 5 & 8 & 2 & 6 & 122 & 122 & 5 & 8 & 2 & 6 & 124 & 4 & 6 & 8 & 8 & 5 & 5 & 5 & 2 & 2 & 6 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 5 & 8 & 4 & 8 & 5 & 8 & 5 & 8 & 5 & 8 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1$	func 7 3 5 11 7 13 14 12 10 3 7 14 5 11 5 6 10 6 12 4 4 8 10 11 6 12 11 10 2 11	0 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	$\begin{array}{c} \dots & C5 \\ 30.33400 \\ 30.33400 \\ 30.33400 \\ 30.33400 \\ 30.33400 \\ 30.33400 \\ 8.78640 \\ 8.78640 \\ 8.78640 \\ 8.78640 \\ 9.20480 \\ 9.20480 \\ 9.20480 \\ 9.20480 \\ 9.20480 \\ 30.33400 \\ 30.3$	0.00000 0.00000	-30.33400 -30.33400 -30.33400 -30.33400 -8.78640 -8.78640 -8.78640 -8.78640 -9.20480 -9.20480 -9.20480 -9.20480 -9.20480 -30.33400 -30.3	0.00000 0.00000	0.00000 0.00000	0.00000 0.00000

2,4,5 trichloroaniline (polarized charges, hexadecane)

-9.20480

0.00000

0.00000

0.00000

;;

;

[moleculetype ; Name C1X] 3	nrexcl							
[atoms] ; nr t; 1	ype ca	resnr 1	residue LIG	atom C	cgnr 1	charge -0.1313	mass 12.000000	typeB	chargeB

0.00000

9.20480

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ca 1 LIG C ha 1 LIG C ca 1 LIG C ca 1 LIG C ca 1 LIG C ca 1 LIG C ha 1 LIG C ca 1 LIG C ca 1 LIG C ca 1 LIG C cl 1 LIG C hn 1 LIG C hn 1 LIG H hn 1 H hn 1 LIG H hn 1	1 2 0.0919 H 3 0.1428 2 4 -0.3018 3 5 0.7270 4 6 -0.4372 7 0.2074 6 -0.0842 1 10 -0.0842 2 11 -0.0842 2 12 -1.1511 2 13 0.4795 3 14 0.4795 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05 3+05 -05	12.00000 1.00000 12.00000 12.00000 12.00000 35.50000 35.50000 35.50000 14.00000 1.00000 1.00000	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 1 1 1 1 1 1 1 1 1 1 1 1 1	1.0551e+02 1.0551e+02 1.0551e+02 1.0070e+02 1.0551e+02 3.3514e+02 5.6216e+02 5.2651e+02 5.00000 -300 00 0.00000 00 0.00000 00 0.00000 00 0.00000 00 0.00000	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.000 0.000 0.000 0.000 0.000

0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

·, ·, ·, ·, ·, ·,

4 4 6 6 7	5 5 5 5 6	12 12 12 12 5	13 14 13 14 12	3 3 3 3 3	8.78640 8.78640 8.78640 8.78640 30.33400	0.00000 0.00000 0.00000 0.00000 0.00000	-8.78640 -8.78640 -8.78640 -8.78640 -30.33400	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
7	6	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	2
1	4	2	3	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
5	8	6	7	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
5	13	12	14	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	2	4	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	8	6	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	8	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	4	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	4	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	1	2	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	2	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	5	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	6	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	4	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	8	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
8	6	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
11	4	5	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	8	2	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
2	5	4	11	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
4	6	5	12	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	6	8	10	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
end											

Lidocaine (gas phase charges)

[moleculetype] ; Name Lidocaine	nrexcl 3
[atoms]	

L atoms	1			_			_		_	
, 11	c yr	a	1 L	IG	C	1	-0.3589	12.000000	o'len	SHOTRED
2	h	a	1 L	IG	H C1	2	0.1836	1.000000		
4	h	a	1 L	IG	H1	4	0.1549	1.000000		
5	0	a	1 L	IG	C2	5	-0.3589	12.000000		
о 7	n C	a	1 L 1 L	IG	C3	6 7	0.1836	12.000000		
8	c	a	1 L	IG	C4	8	-0.0235	12.000000		
9 10	c	a 3	1 L 1 L	IG	C5 C6	9 10	-0.3112	12.000000		
11	h	.c	1 L	IG	H3	11	0.0898	1.000000		
13	h	.C	1 L	IG	H4 H5	13	0.0898	1.000000		
14 15	C	3	1 L 1 I	IG	C7 H6	14 15	-0.3112	12.000000		
16	h	.c	1 L	IG	H7	16	0.0898	1.000000		
17 18	h	.C n	1 I 1 I	IG	H8 N	17 18	0.0898	1.000000		
19	h	n	1 I	IG	H9	19	0.3223	1.000000		
20 21		с 0	1 L 1 L	IG IG	C8 0	20 21	0.6026	12.000000		
22	c	3	1 L	IG	C9	22	0.1477	12.000000		
23 24	h	.1	1 L 1 L	IG	H10 H11	23 24	-0.0093	1.000000		
25	n	.3	1 L	IG	N1	25	-0.1523	14.000000		
26 27	c h	3	1 L 1 L	IG IG	C10 H12	26 27	-0.0178 0.0456	12.000000		
28	h	.1	1 L	IG	H13	28	0.0456	1.000000		
29 30	c h	3 .C	1 L 1 L	IG	H14	29 30	0.0569	1.000000		
31	h	.c	1 L	IG	H15	31	0.0569	1.000000		
32	n	.c 3	1 L 1 L	IG	C12	32 33	-0.0569	12.000000		
34	h	1	1 L	IG	H17	34	0.0456	1.000000		
35 36	n c	3	1 L 1 L	IG	C13	35 36	-0.1914	12.000000		
37	h	.c	1 L	IG	H19 H20	37	0.0569	1.000000		
39	h	.c	1 I	IG	H21	39	0.0569	1.000000		
[bonds]									
; ai 1	aj func 2	trk 1 1.08	c 370e-01	2.	8811e+05					
3	4	1 1.08	370e-01	2.	8811e+05					
10	11	1 1.00	920e-01	2.	8225e+05					
10	12	1 1.09	920e-01	2.	8225e+05					
10	15	1 1.09	920e-01 920e-01	2.	8225e+05					
14	16 17	1 1.09	20e-01	2.	8225e+05					
18	19	1 1.00)90e-01	3.	4326e+05					
22 22	23 24	1 1.09	930e-01	2.	8108e+05					
26	27	1 1.09	930e-01	2.	8108e+05					
26 29	28 30	1 1.09)30e-01	2.	8108e+05 8225e+05					
29	31	1 1.09	20e-01	2.	8225e+05					
29 33	32 34	1 1.09	920e-01 930e-01	2.	8225e+05 8108e+05					
33	35	1 1.09	30e-01	2.	8108e+05					
36 36	37 38	1 1.09	920e-01 920e-01	2.	8225e+05 8225e+05					
36	39	1 1.09	20e-01	2.	8225e+05					
1	3 9	1 1.38	370e-01 370e-01	4.	0033e+05 0033e+05					
3	5	1 1.38	870e-01	4.	0033e+05					
5 7	8	1 1.38	870e-01	4.	0033e+05					
7	14	1 1.51	30e-01	2.	7070e+05					
8 8	9 18	1 1.42	220e-01	4. 3.	1154e+05					
9 19	10	1 1.51	130e-01	2.	7070e+05					
20	20	1 1.21	40e-01	4. 5.	4225e+05					
20	22 25	1 1.50)80e-01	2.	7472e+05					
25	26	1 1.47	700e-01	2.	6828e+05					
25 26	33 29	1 1.47	700e-01	2.	6828e+05					
33	36	1 1.53	350e-01	2.	5363e+05					

[pairs]

;	ai 1	aj fur	lct	1			
	1	11		1			
	1	12		1			
	2	4 5		1 1			
	2 2	8 10		1 1			
	9	4		1			
	4	7		1			
	5 5	15 16		1 1			
	5 6	17 8		1 1			
	6	14 19		1			
	8	15		1			
	8	16		1			
	8 8	11 12		1 1			
	8 9	13 19		1 1			
	18 18	23		1			
	19	21		1			
	19 21	22		1			
	21 22	24 27		1 1			
	22 22	28 34		1 1			
	22	35		1			
	23	33		1			
	24	33		1			
	25 25	30 31		1 1			
	25 25	32 37		1 1			
	25 25	38 39		1 1			
	26	34 35		1			
	27	33		1			
	27 27	30 31		1 1			
	27 28	32 33		1 1			
	28 28	30 31		1 1			
	28	32		1			
	34	38		1			
	34 35	39 37		1			
	35 35	38 39		1 1			
	1 1	7 18		1 1			
	3	8		1			
	3	14		1			
	5	18		1			
	7	10 20		1 1			
	8 8	21 22		1 1			
	9 9	14 20		1 1			
	10 14	18 18		1			
	18	25		1			
	20 20	20 33		1			
	21 22	25 29		1			
	22 26	36 36		1 1			
	29	33		1			
[;	angles ai] aj	ak	fun	ct	theta cth	
	1 2	3 1	4 3		1 1	1.2001e+02 1.2001e+02	4.0551e+02 4.0551e+02
	2 3	1 5	9 6		1 1	1.2001e+02 1.2001e+02	4.0551e+02 4.0551e+02
			-			· · · -	=

[dihedrals]

Ľά	Tuec	irais j										
;i	j	k l		func	CO	C5						
	1	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	1	9	10	11	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	1	9	10	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	1	9	10	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	2	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	2	1	3	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	2	1	9	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	2	1	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	9	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	4	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	4	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	5	7	14	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	5	7	14	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	5	7	14	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	6	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	6	5	7	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	7	8	18	19	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
	8	7	14	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	7	14	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	7	14	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	9	10	11	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	9	10	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	9	10	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;

9 18 18 19 19	8 20 20 18 18	18 22 22 20 20	19 23 24 21 22	3 3 3 3 3 3	3.76560 0.00000 0.00000 29.28800 20.92000	0.00000 0.00000 -8.36800 0.00000	-3.76560 0.00000 0.00000 -20.92000 -20.92000	0.00000 0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000 0.00000	$\begin{array}{c} 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ \end{array}$;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
21 21 22 22	20 20 25 25	22 22 26 26	23 24 27 28	3333	3.68192 3.68192 1.25520 1.25520	-4.35136 -4.35136 3.76560 3.76560	0.00000 0.00000 0.00000 0.00000	1.33888 1.33888 -5.02080 -5.02080	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , ,
22 22 23 23 24	25 25 22 22 22	33 25 25 25	35 26 33 26	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	1.25520 1.25520 1.25520 1.25520 1.25520	3.76560 3.76560 3.76560 3.76560	0.00000 0.00000 0.00000 0.00000	-5.02080 -5.02080 -5.02080 -5.02080 -5.02080	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , , ,
24 25 25 25	22 26 26 26	25 29 29 29	33 30 31 32	3 3 3 3 3	1.25520 0.65270 0.65270 0.65270	3.76560 1.95811 1.95811 1.95811	0.00000 0.00000 0.00000 0.00000	-5.02080 -2.61082 -2.61082 -2.61082	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	2 2 2 2 2 2 2
25 25 25 26	33 33 33 25	36 36 36 33	37 38 39 34	3 3 3 3	0.65270 0.65270 0.65270 1.25520	1.95811 1.95811 1.95811 3.76560	0.00000 0.00000 0.00000 0.00000	-2.61082 -2.61082 -2.61082 -5.02080	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , , , , ,
26 27 27 27 27	25 26 26 26	33 25 29 29	35 33 30 31	3333	1.25520 1.25520 0.65270 0.65270	3.76560 3.76560 1.95811 1.95811	0.00000 0.00000 0.00000 0.00000	-5.02080 -5.02080 -2.61082 -2.61082	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
27 28 28 28 28 28	26 26 26 26 26	29 25 29 29 29	32 33 30 31 32	3 3 3 3 3 3	0.65270 1.25520 0.65270 0.65270 0.65270	1.95811 3.76560 1.95811 1.95811 1.95811	0.00000 0.00000 0.00000 0.00000	-2.61082 -5.02080 -2.61082 -2.61082 -2.61082	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	· · · ·
34 34 34 35	33 33 33 33	36 36 36 36	37 38 39 37	3 3 3 3	0.65270 0.65270 0.65270 0.65270 0.65270	1.95811 1.95811 1.95811 1.95811 1.95811	0.00000 0.00000 0.00000 0.00000	-2.61082 -2.61082 -2.61082 -2.61082 -2.61082	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , , , ,
35 35 2 1	33 33 1 5	36 36 9 3	38 39 3 4	3 3 3 3	0.65270 0.65270 9.20480 9.20480	$\begin{array}{c} 1.95811 \\ 1.95811 \\ 0.00000 \\ 0.00000 \end{array}$	0.00000 0.00000 -9.20480 -9.20480	-2.61082 -2.61082 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	· · · · · · · · · · · · · · · · · · ·
3 20 1 1 1	7 8 3 9 9	5 18 5 8 8	6 19 7 7 18	3 3 3 3 3 3 3	9.20480 9.20480 30.33400 30.33400 30.33400	0.00000 0.00000 0.00000 0.00000	-9.20480 -9.20480 -30.33400 -30.33400 -30.33400	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	· · · · ·
3 3 3 3	1 1 5 5	9 9 7 7	8 10 8 14	3 3 3 3	30.33400 30.33400 30.33400 30.33400 30.33400	0.00000 0.00000 0.00000 0.00000	-30.33400 -30.33400 -30.33400 -30.33400	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	3 • • • •
9 5 5 7	1 7 7 8	3 8 8 9	5 9 18 10	3 3 3 3	30.33400 30.33400 30.33400 30.33400	0.00000 0.00000 0.00000 0.00000	-30.33400 -30.33400 -30.33400 -30.33400	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , , , , ,
7 8 9 9	8 18 18 8	18 20 20 7	20 21 22 14	3333	3.76560 20.92000 20.92000 30.33400	0.00000 0.00000 0.00000 0.00000	-3.76560 -20.92000 -20.92000 -30.33400	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	;; ;; ;
9 10 14 18 20	9 7 20 22	18 8 8 22 25	18 18 25 26	3 3 3 3 3 3	30.33400 30.33400 0.00000 1.25520	0.00000 0.00000 0.00000 3.76560	-30.33400 -30.33400 0.00000 0.00000	0.00000 0.00000 0.00000 -5.02080	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , , , ,
20 21 22 22	22 20 25 25	25 22 26 33	33 25 29 36	3 3 3 3 3	1.25520 0.00000 5.27184 5.27184	3.76560 0.00000 3.76560 3.76560	$\begin{array}{c} 0.00000\\ 0.00000\\ -4.01664\\ -4.01664\end{array}$	-5.02080 0.00000 -5.02080 -5.02080	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	· · · · ·
26 29 5 7	25 26 8 9	33 25 7 8	36 33 14 18	3333	5.27184 5.27184 9.20480 9.20480	3.76560 3.76560 0.00000 0.00000	-4.01664 -4.01664 -9.20480 -9.20480	-5.02080 -5.02080 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	0.00000 0.00000 0.00000 0.00000	, , , , ,
22 end	18	9 20	° 21	3 3	9.20480 87.86400	0.00000	-9.20480 -87.86400	0.00000	0.00000	0.00000	; ;

Lidocaine (polarized charges, water)

[moleculet ; Name Lidocaine	ype]	nrexcl 3							
[atoms]									
; nr	type	resnr	residue	atom	cgnr	charge	mass	typeB	chargeB
1	ca	1	LIG	С	Ū 1	-0.38580	12.000000	• •	•
2	ha	1	LIG	Н	2	0.20260	1.000000		
3	ca	1	LIG	C1	3	-0.10160	12.000000		
4	ha	1	LIG	H1	4	0.17180	1.000000		
5	ca	1	LIG	C2	5	-0.38580	12.000000		
6	ha	1	LIG	H2	6	0.20260	1.000000		
7	ca	1	LIG	C3	7	0.23220	12.000000		
8	ca	1	LIG	C4	8	-0.01690	12.000000		
9	ca	1	LIG	C5	9	0.25190	12.000000		

	$\begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 39 \end{array}$	c3 hc hc c3 hc hc c3 hc hc hc hc hc hc hc hc hc hc hc hc hc	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	LIG LIG LIG LIG LIG LIG LIG LIG LIG LIG	C6 H3 H4 H5 C7 H6 H7 H8 N H9 C8 C9 H10 H11 N10 H12 H13 C114 H15 H16 C19 H11 H13 C114 H15 H16 C12 H17 H18 C16 H17 H18 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H19 C16 H17 H11 N10 H111 H11 C16 H17 H19 C16 H111 H11 C16 H17 H19 C16 H111 H11 C16 H112 H112 H112 H112 H112 H112 H112 H1	$\begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 20\\ 21\\ 22\\ 23\\ 24\\ 25\\ 26\\ 27\\ 28\\ 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 38\\ 39 \end{array}$	$\begin{array}{c} -0.29650\\ 0.08960\\ 0.08960\\ 0.08960\\ 0.08960\\ 0.08960\\ 0.08960\\ 0.08960\\ 0.3750\\ 0.64440\\ 0.3750\\ 0.64440\\ 0.04750\\ 0.04750\\ 0.04750\\ 0.04750\\ 0.04750\\ 0.05780\\ 0.05780\\ 0.05780\\ 0.04720\\ 0.04720\\ 0.04720\\ 0.05780\\ 0.05780\\ 0.05780\\ 0.05780\\ 0.0472$	$\begin{array}{c} 12.000000\\ 1.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 12.00000\\ 12.00000\\ 12.00000\\ 12.00000\\ 1.00000\\ 12.00000\\ 1.00000\\ 12.00000\\ 1.00000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.00000\\ 0.000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.000\\ 0.000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.000\\ 0.000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.000\\ 0.000\\ 0.000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.000\\ 0.000\\ 0.000\\ 0.0000\\ 0.$
C ;	bonds ai 1 3 5 10 10 10 14 14 14 18 22 26 26 29 29 33 36 36 1 1 3 5 7 7 8 8 9 18 20 22 25 25 26 33] aj funct 2 1 4 1 6 1 11 1 12 1 13 1 15 1 16 1 17 1 19 1 23 1 24 1 17 1 19 1 23 1 24 1 30 1 31 1 32 1 34 1 35 1 37 1 38 1 39 1 37 1 38 1 39 1 37 1 38 1 1 9 1 1 5 1 1 7 1 1 9 1 23 1 1 24 1 1 1 27 1 1 28 1 29 1 36 1	r k 1.0870e-(1.0870e-(1.0870e-(1.0920e-(1.0920e-(1.0920e-(1.0920e-(1.0930e-(1.3870	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8811e+05 8811e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8108e+05 8108e+05 8108e+05 8108e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 0033e+05 0033e+05 0033e+05 0033e+05 1154e+05 7070e+05 0033e+05 7070e+05 0033e+05 5363e+05 5363e+05 5363e+05			
[;	pairs ai 1 1 2 2 2 9 4 5 5 5 6 6] aj funct 6 11 12 13 4 5 8 10 4 6 7 15 16 17 8 14	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1					

[;;	
angles ai 1 2 3 4 6 7 7 7 8 9 9 9 11 11 12 15 15 16 19 20	$\begin{array}{c} 7\\ 8\\ 8\\ 8\\ 8\\ 8\\ 9\\ 18\\ 19\\ 21\\ 22\\ 22\\ 22\\ 23\\ 24\\ 42\\ 25\\ 25\\ 25\\ 25\\ 25\\ 25\\ 25\\ 25\\ 25\\ 2$
] j j 3 1 1 5 3 5 14 14 18 10 10 10 10 10 10 10 11 4 14 18 22	$\begin{array}{c} 19\\ 15\\ 16\\ 17\\ 1\\ 12\\ 23\\ 24\\ 12\\ 23\\ 24\\ 22\\ 24\\ 22\\ 24\\ 22\\ 24\\ 22\\ 23\\ 35\\ 26\\ 33\\ 0\\ 31\\ 23\\ 33\\ 33\\ 33\\ 33\\ 33\\ 33\\ 33\\ 33\\ 33$
ak funct 4 1 3 1 9 1 6 1 7 1 15 1 16 1 17 1 19 1 11 1 12 1 13 1 16 1 17 1 20 1 23 1	111111111111111111111111111111111111111
theta cth 1.2001e+02 1.2001e+02 1.2001e+02 1.2001e+02 1.2001e+02 1.2001e+02 1.1015e+02 1.1015e+02 1.1015e+02 1.1015e+02 1.1015e+02 1.0835e	
4.0551e+02 4.0551e+02 4.0551e+02 4.0551e+02 4.0551e+02 3.9296e+02 3.9296e+02 3.9296e+02 3.9296e+02 3.9296e+02 3.9296e+02 3.9296e+02 3.2995e+02 3.2995e+02 3.2995e+02 3.2995e+02 3.2995e+02 3.2995e+02 3.2995e+02 3.9857e+02	

20	22	24	1	1.0766e+02	3.9857e+02
23	22	24	1	1.0955e+02	3.2786e+02
23	22	25	1	1.0992e+02	4.1330e+02
24	22	25	1	1.0992e+02	4.1330e+02
25	26	27	1	1.0992e+02	4.1330e+02
25	26	28	1	1.0992e+02	4.1330e+02
25	33	34	1	1.0992e+02	4.1330e+02
25	33	35	1	1.0992e+02	4.1330e+02
26	29	30	1	1.1005e+02	3.8802e+02
26	29	31	1	1.1005e+02	3.8802e+02
26	29	32	1	1.1005e+02	3.8802e+02
27	26	28	1	1.0955e+02	3.2786e+02
27	26	29	1	1.1007e+02	3.8794e+02
28	26	29	1	1.1007e+02	3.8794e+02
30	29	31	1	1.0835e+02	3.2995e+02
30	29	32	1	1.0835e+02	3.2995e+02
31	29	32	1	1.0835e+02	3.2995e+02
33	36	37	1	1.1005e+02	3.8802e+02
33	36	38	1	1.1005e+02	3.8802e+02
33	36	39	1	1.1005e+02	3.8802e+02
34	33	35	1	1.0955e+02	3.2786e+02
34	33	36	1	1.1007e+02	3.8794e+02
35	33	36	1	1.1007e+02	3.8794e+02
37	36	38	1	1.0835e+02	3.2995e+02
37	36	39	1	1.0835e+02	3.2995e+02
38	36	39	1	1.0835e+02	3.2995e+02
1	3	5	1	1.1997e+02	5.6216e+02
1	9	8	1	1.1997e+02	5.6216e+02
1	9	10	1	1.2063e+02	5.3421e+02
3	1	9	1	1.1997e+02	5.6216e+02
3	5	7	1	1.1997e+02	5.6216e+02
5	7	8	1	1.1997e+02	5.6216e+02
5	7	14	1	1.2063e+02	5.3421e+02
7	8	9	1	1.1997e+02	5.6216e+02
7	8	18	1	1.1989e+02	5.6877e+02
8	7	14	1	1.2063e+02	5.3421e+02
8	9	10	1	1.2063e+02	5.3421e+02
8	18	20	1	1.2371e+02	5.3798e+02
9	8	18	1	1.1989e+02	5.6877e+02
18	20	21	1	1.2203e+02	6.3455e+02
18	20	22	1	1.1515e+02	5.6785e+02
20	22	25	1	1.1114e+02	5.5723e+02
21	20	22	1	1.2311e+02	5.6928e+02
22	25	26	1	1.1090e+02	5.3564e+02
22	25	33	1	1.1090e+02	5.3564e+02
25	26	29	1	1.1038e+02	5.5379e+02
25	33	36	1	1.1038e+02	5.5379e+02
26	25	33	1	1.1090e+02	5.3564e+02

[dihed	drals]]									
;i j	k 1		func	CO	C5						
1	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
1	9	10	11	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
1	9	10	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
1	9	10	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
2	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	3	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	9	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
2	1	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
9	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
5	7	14	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
5	7	14	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
5	7	14	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
6	5	7	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
7	8	18	19	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
8	7	14	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
8	7	14	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
8	7	14	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
8	9	10	11	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
8	9	10	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
8	9	10	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
9	8	18	19	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
18	20	22	23	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
18	20	22	24	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
19	18	20	21	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
19	18	20	22	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
21	20	22	23	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
21	20	22	24	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
22	25	26	27	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
22	25	26	28	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
22	25	33	34	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
22	25	33	35	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
23	22	25	26	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
23	22	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
24	22	25	26	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
24	22	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
25	26	29	30	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
25	26	29	31	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;

25	26	29	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
25	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
25	33	36	38	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
25	33	36	39	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
26	25	33	34	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
26	25	33	35	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
27	26	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
27	26	29	30	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
27	26	29	31	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
27	26	29	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
28	26	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
28	26	29	30	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
28	26	29	31	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
28	26	29	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
34	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
34	33	36	38	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
34	33	36	39	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
35	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
35	33	36	38	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
35	33	36	39	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
∠ 1	L L	3	3	2	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
2	5 7	5	4	2	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
3	6	10	10	2	9.20400	0.00000	-9.20460	0.00000	0.00000	0.00000	,
20	0 2	10	19	2	9.20400	0.00000	-20 22400	0.00000	0.00000	0.00000	,
1	3	0	7	2	20.22400	0.00000	-30.33400	0.00000	0.00000	0.00000	,
1	9	0	10	2	20.22400	0.00000	-30.33400	0.00000	0.00000	0.00000	,
3	9	0	010	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	,
3	1	9	0 10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	,
3	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	?
3	5	7	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	?
q	1	3	5	3	30 33400	0.00000	-30 33400	0.00000	0.00000	0.00000	?
5	7	8	g	3	30 33400	0.00000	-30 33400	0.00000	0.00000	0.00000	?
5	7	8	18	3	30 33400	0.00000	-30 33400	0.00000	0.00000	0.00000	?
7	Ŕ	ğ	10	3	30 33400	0.00000	-30 33400	0.00000	0.00000	0.00000	?
7	8	18	20	3	3 76560	0.00000	-3 76560	0.00000	0.00000	0.00000	:
8	18	20	21	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
8	18	20	22	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
9	8	7	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	:
9	8	18	20	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	:
10	9	8	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	:
14	7	8	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	÷
18	20	22	25	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	÷
20	22	25	26	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	÷
20	22	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
21	20	22	25	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
22	25	26	29	3	5.27184	3.76560	-4.01664	-5.02080	0.00000	0.00000	;
22	25	33	36	3	5.27184	3.76560	-4.01664	-5.02080	0.00000	0.00000	;
26	25	33	36	3	5.27184	3.76560	-4.01664	-5.02080	0.00000	0.00000	;
29	26	25	33	3	5.27184	3.76560	-4.01664	-5.02080	0.00000	0.00000	;
5	8	7	14	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
7	9	8	18	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
10	1	9	8	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
22	18	20	21	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;

end----- Lidocaine (polarized charges, hexadecane)

[molecu ; Name Lidocair	letype] Ne	nrexcl 3							
[atoms]								
; nr	type	resnr	residue	atom	cgnr	charge	mass	typeB	chargeB
1	ca	1	LIG	С	1	-0.3681	12.000000	••	•
2	ha	1	LIG	Н	2	0.1902	1.000000		
3	ca	1	LIG	C1	3	-0.0927	12.000000		
4	ha	1	LIG	H1	4	0.1608	1.000000		
5	ca	1	LIG	C2	5	-0.3681	12.000000		
6	ha	1	LIG	H2	6	0.1902	1.000000		
7	ca	1	LIG	C3	7	0.2372	12.000000		
8	ca	1	LIG	C4	8	-0.0200	12.000000		
9	ca	1	LIG	C5	9	0.2451	12.000000		
10	c3	1	LIG	C6	10	-0.3072	12.000000		
11	hc	1	LIG	HЗ	11	0.0902	1.000000		
12	hc	1	LIG	H4	12	0.0902	1.000000		
13	hc	1	LIG	H5	13	0.0902	1.000000		
14	c3	1	LIG	C7	14	-0.3072	12.000000		
15	hc	1	LIG	H6	15	0.0902	1.000000		
16	hc	1	LIG	H7	16	0.0902	1.000000		
17	hc	1	LIG	H8	17	0.0902	1.000000		
18	n	1	LIG	N	18	-0.4665	14.000000		
19	hn	1	LIG	Н9	19	0.3287	1.000000		
20	с	1	LIG	C8	20	0.6213	12.000000		
21	0	1	LIG	0	21	-0.6684	16.000000		
22	c3	1	LIG	C9	22	0.1071	12.000000		
23	h1	1	LIG	H10	23	0.0073	1.000000		
24	h1	1	LIG	H11	24	0.0073	1.000000		
25	n3	1	LIG	N1	25	-0.1512	14.000000		
26	c3	1	LIG	C10	26	-0.0300	12.000000		

27 28 29 30 31 32 33 34 35 36	h1 h1 c3 hc hc hc c3 h1 h1 c3	1 1 1 1 1 1 1 1 1	LIG LIG LIG LIG LIG LIG LIG LIG	H12 H13 C11 H14 H15 H16 C12 H17 H18 C13	27 28 29 30 31 32 33 34 35 36	$\begin{array}{c} 0.0506\\ 0.0506\\ -0.1755\\ 0.0536\\ 0.0536\\ -0.0300\\ 0.0506\\ 0.0506\\ -0.1755\end{array}$	$\begin{array}{c} 1.000000\\ 1.00000\\ 12.00000\\ 1.00000\\ 1.00000\\ 1.00000\\ 12.00000\\ 12.00000\\ 1.00000\\ 1.00000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.0000\\ 12.000\\$
37 38 39	hc hc hc	1 1 1	LIG LIG LIG	H19 H20 H21	37 38 39	0.0536 0.0536 0.0536	1.000000 1.000000 1.000000
; ai ; ai 1 3 5 10 10 10 14 14 14 14 14 14 14 14 14 14	aj funct 2 1 4 1 2 1 12 1 11 1 12 1 13 1 15 1 15 1 16 1 17 1 23 1 23 1 24 1 27 1 23 1 30 1 31 1 31 1 32 1 31 1 32 1 33 1 35 1 37 1 35 1 37 1 35 1 37 1 35 1 1 3 1 1 37 1 35 1 1 3 1 1 35 1 1 1 31 1 35 1 1 3 1 1 35 1 1 3 1 1 35 1 1 1 35 1 1 3 1 1 35 1 1 3 3 1 9 1 1 2 1 1 22 1 22 1 22 1 25 1 1 2 1 1 22 1 25 1 1 2 1 1 22 1 25 1 1 2 1 1 22 1 22 1 25 1 1 2 1 1 22 1 22 1 25 1 21 1 22 1 22 1 25 1 33 1 39 1 39 1 39 1 32 1 39 1 32 1 32 1 33 1 9 1 32 1 32 1 33 1 9 1 32 1 33 1 39 1 32 1 33 1 39 1 32 1 33 1 21 1 22 1 225 1 23 1 33 1 33 1 33 1 33 1 39 1 32 1 32 1 33 1 33 1 39 1 32 1 33 1 39 1 32 1 32 1 33 1 33 1 33 1 39 1 32 1 33 1 33 1 33 1 33 1 33 1 33 1 33 1 39 1 33 1 33 1 33 1 33 1 32 1 33 1	r k 1.0870e 1.0870e 1.0870e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0920e 1.0930e 1.0930e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0930e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0930e 1.0920e 1.0930e 1.0930e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0920e 1.0930e 1.0920e 1.0920e 1.0920e 1.3870e 1.3870e 1.3870e 1.3870e 1.3870e 1.4200e 1.4700e 1.4700e 1.4700e 1.5350e	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8811e+05 8811e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8108e+05 8108e+05 8108e+05 8108e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 8225e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0033e+05 0036e+05 8225e+05 8256e+			
<pre>[pairs] ; ai 1 1 1 2 2 2 2 9 4 4 5 5 6 6 7 8 8 8 8 9 18 19 19 21 22 22 22 22 2 </pre>] aj funct 6 11 12 13 4 5 8 10 4 6 7 15 16 17 15 16 17 11 19 15 16 17 11 19 23 24 21 22 23 24 27 28 34	$1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\$					

28 33 1 28 30 1 28 31 1 34 37 1 34 37 1 34 39 1 35 37 1 35 39 1 1 7 1 3 1 8 1 3 10 1 3 14 1 9 5 1 7 10 1 7 20 1 8 21 1 8 22 1 9 14 1 1 8 1 1 7 20 1 7 10 1 7 20 1 8 21 1 8 22 1 9 14 1 1 8 1 1 8 25 1 20 26 1 20 33 1 21 25 1 22 36 1 23 5 1 21 25 1 22 29 1 22 36 1 22 36 1 23 5 1 21 25 1 22 36 2 1 3 1 1.2001+02 4.055 3 5 6 1 1.2001+02 4.055 3 5 6 1 1.2001+02 4.055 3 5 6 1 1.2001+02 4.055 5 7 14 15 1 1.1015+02 3.929 7 14 15 1 1.1015+02 3.929 7 14 17 1 1.1015+02 3.929 7 14 17 1 1.1015+02 3.929 9 10 12 1 1.1015+02 3.929 9 10 13 1 1.0015+02 3.929 9 10 13 1 1.0015+02 3.929 9 10 12 1 1.0015+02 3.929 9 10 13 1 1.0015+02 3.929 11 10 12 1 .0035+02 3.299 11 10 12 1 .0035+02 3.299 11 10 12 1 .0035+02 3.299 15 14 16 1 1.0015+02 3.299 15 14 16 1 1.0035+02 3.299 15 14 16 1 1.0015+02 3.299 15 14 16 1 1.005+02 3.299 15 14 1.005+02 3.299 15 14 1.005+02 3.380 26 29 30 1 1.1005+02 3.880 26 29 30 1 1.10

~~	~ ~	07		4 4005 100	0 0000 .00
33	36	37	1	1.1005e+02	3.8802e+02
33	36	38	1	1.1005e+02	3.8802e+02
33	36	39	1	1.1005e+02	3.8802e+02
34	33	35	1	1.0955e+02	3.2786e+02
34	33	36	1	1.1007e+02	3.8794e+02
35	33	36	1	1.1007e+02	3.8794e+02
37	36	38	1	1.0835e+02	3.2995e+02
37	36	39	1	1.0835e+02	3.2995e+02
38	36	39	1	1.0835e+02	3.2995e+02
1	3	5	1	1 1997e+02	5 6216e+02
1	ğ	Ř	1	1 1997e+02	5 6216e+02
1	ă	10	1	1 20630+02	5 34210+02
à	1	ĨĞ	1	1 1997+02	5 62160+02
3	Ē	7	1	1.10070+02	5.62160+02
5	7	Ŕ	1	1 10070+02	5.02100+02 5.62160+02
5	7	14	1	1 20630+02	5 3/2104-02
7	6	14	1	1.2003e+02	5.54210+02
4	°.	10	1	1.19970+02	5.62160+02
1	8	18	1	1.1989e+02	5.68//e+02
8	(14	1	1.2063e+02	5.3421e+02
8	9	10	1	1.2063e+02	5.3421e+02
8	18	20	1	1.2371e+02	5.3798e+02
9	8	18	1	1.1989e+02	5.6877e+02
18	20	21	1	1.2203e+02	6.3455e+02
18	20	22	1	1.1515e+02	5.6785e+02
20	22	25	1	1.1114e+02	5.5723e+02
21	20	22	1	1.2311e+02	5.6928e+02
22	25	26	1	1.1090e+02	5.3564e+02
22	25	33	1	1.1090e+02	5.3564e+02
25	26	29	1	1.1038e+02	5.5379e+02
25	33	36	1	1.1038e+02	5.5379e+02
26	25	33	1	1.1090e+02	5.3564e+02

[dihedrals]

;i	j	k l		func	CO	C5						
	1	3	5	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	1	9	10	11	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	1	9	10	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	1	9	10	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	2	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	
	2	1	3	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	÷
	2	1	ğ	Ř	3	30 33400	0 00000	-30 33400	0 00000	0 00000	0 00000	?
	2	1	ă	10	ž	30 33400	0,00000	-30 33400	0.00000	0.00000	0.00000	:
	ā	1	ž	10	3	30 33400	0.00000	-30 33400	0.00000	0.00000	0.00000	?
	1	2	5	Ē	2	20.22400	0.00000	-20.22400	0.00000	0.00000	0.00000	?
	4	2	5	7	2	20.22400	0.00000	-30.33400	0.00000	0.00000	0.00000	?
	4	37	11	15	2	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	,
	5	4	14	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	5	<u>/</u>	14	10	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	5	<u>′</u>	14	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	6	5	2	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	6	5	7	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
	7	8	18	19	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;
	8	7	14	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	7	14	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	7	14	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	9	10	11	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	9	10	12	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	8	9	10	13	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	9	8	18	19	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	:
	18	20	22	23	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
	18	20	22	24	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	:
	19	18	20	21	3	29,28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	÷
	19	18	20	22	3	20.92000	0.00000	-20,92000	0.00000	0.00000	0.00000	
	21	20	22	23	3	3 68192	-4 35136	0 00000	1 33888	0 00000	0 00000	?
	21	20	22	24	ž	3 68192	-4 35136	0.00000	1 33888	0.00000	0.00000	:
	22	25	26	27	ž	1 25520	3 76560	0.00000	-5 02080	0.00000	0.00000	:
	22	25	20	28	3	1 25520	3 76560	0.00000	-5 02080	0.00000	0.00000	?
	22	25	20	3/	3	1 25520	3 76560	0.00000	-5 02080	0.00000	0.00000	?
	22	25	33	35	3	1 25520	3 76560	0.00000	-5 02080	0.00000	0.00000	?
	22	20	25	26	3	1.25520	3 76560	0.00000	-5 02080	0.00000	0.00000	?
	23	22	20	20	2	1.25520	3.70500	0.00000	-5.02080	0.00000	0.00000	,
	23	22	25	33	3	1.25520	3.70500	0.00000	-5.02080	0.00000	0.00000	;
	24	22	25	20	3	1.25520	3.70500	0.00000	-5.02080	0.00000	0.00000	;
	24	22	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
	25	26	29	30	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	25	26	29	31	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	25	26	29	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	25	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	25	33	36	38	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	25	33	36	39	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	26	25	33	34	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
	26	25	33	35	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
	27	26	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;
	27	26	29	30	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	27	26	29	31	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	27	26	29	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	28	26	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	
	28	26	29	30	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
	28	26	29	31	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	÷
	28	26	29	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	:
	34	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	:
	34	33	36	38	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	÷
	34	33	36	39	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	:
					-							,

35	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;	
35	33	36	38	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;	
35	33	36	39	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;	
2	Ţ	9	3	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
1	5	2	4	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
3	6	5	5	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
20	0	10	19	3	9.20460	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
1	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
1	9	0	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
1	9	0	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
3	1	9	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
3	Ţ	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
3	5	1	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
3	5	1	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
9	17	3	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
5	7	0	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
5	6	8	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
7	8	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
1	8	18	20	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;	
8	18	20	21	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;	
0	10	20	14	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;	
9	8	10	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
9	8	18	20	3	3.76560	0.00000	-3.76560	0.00000	0.00000	0.00000	;	
10	9	õ	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
14	60	8	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;	
18	20	22	25	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;	
20	22	25	26	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;	
20	22	25	33	3	1.25520	3.76560	0.00000	-5.02080	0.00000	0.00000	;	
21	20	22	25	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;	
22	25	20	29	3	5.27104	3.70000	-4.01664	-5.02080	0.00000	0.00000	;	
22	25	33	30	3	5.27104	3.70500	-4.01004	-5.02080	0.00000	0.00000	;	
26	25	33	30	3	5.27184	3.76560	-4.01664	-5.02080	0.00000	0.00000	;	
29	26	25	33	3	5.27184	3.76560	-4.01664	-5.02080	0.00000	0.00000	;	
5	ŏ	(14	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
10	9	ŏ	18	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
10	10	9	8 01	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;	
22	18	20	21	3	01.00400	0.00000	-01.00400	0.00000	0.00000	0.00000	;	
and												
ena												

Methanol (gas phase charges)

[molecul ; Name Methanol	Letype]	nrexcl 3										
[atoms] ; nr 2 3 4 5 6	l t:	ype c3 h1 h1 h1 oh ho	resnr 1 1 1 1 1 1	residue LIG LIG LIG LIG LIG LIG	e atom C H H1 H2 O H3	cgn	r chi 1 0.1 2 0.0 3 0.0 4 0.0 5 -0.6 6 0.3	arge 615 194 194 194 019 822	mas 12.000000 1.000000 1.000000 16.000000 1.000000	s typeB	chargeB		
[bonds] ; ai 1 1 5 1	aj fu 2 3 4 6 5	nct 1 1 1 1	r k 1.0930 1.0930 1.0930 9.7400 1.4260	0e-01 2 0e-01 2 0e-01 2 0e-02 3 0e-01 2	2.8108e- 2.8108e- 2.8108e- 3.0928e- 2.6284e-	+05 +05 +05 +05 +05							
[pairs] ; ai 2 3 4	aj fu 6 6 6	nct	1 1 1										
[angles ; ai 2 2 2 3 3 4] aj 5 1 1 1 1 1	ak 6 3 4 5 4 5 5	funct 1 1 1 1 1 1	theta 1.08166 1.09556 1.09586 1.09886 1.09886 1.09886 1.09886	cth e+02 3 e+02 3 e+02 3 e+02 3 e+02 4 e+02 4 e+02 4 e+02 4	.9405e .2786e .2786e .2652e .2652e .2652e .2652e	+02 +02 +02 +02 +02 +02 +02 +02						
[dihedra ;i j k 2 3 4	als] 1 1 1 1	5 5 5	func 6 6 6	CO 3 3 3	. C5 0.69873 0.69873 0.69873	3 : 3 : 3 :	2.09618 2.09618 2.09618	() ()	0.00000 0.00000 0.00000	-2.79491 -2.79491 -2.79491	0.00000 0.00000 0.00000	0.00000 0.00000 0.00000	;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
end						Meths	anol (n/	alar	ized cha	rges wat	a r)		
end [molecul ; Name Methanol	Letype	ן	nrexcl 3			Metha	anol (po	olar	ized cha	rges, wat	er)		
<pre>end [molecul ; Name Methanol [atoms] ; nr 1 2 3 4 5 6</pre>	Letype t) c3 h1 h1 h1 h0	nrexcl 3 resnr 1 1 1 1 1	residue LIG LIG LIG LIG LIG LIG	e atom C H1 H2 O H3	cgn	r chi 1 0.22 2 0.0 3 0.0 5 -0.63 6 0.4	arge 049 189 189 903 287	mas 12.000000 1.000000 1.000000 1.000000 1.000000 1.000000	rges, wat	er) chargeB		
<pre>end [molecul ; Name Methanol [atoms] ; nr</pre>	Letype t aj fu 3 4 6 5) c3 h1 h1 h1 h0 h0 nct 1 1 1 1	nrexcl 3 resnr 1 1 1 1 1 1 1 1 1 1 0933 1.0933 1.0933 9.7400 1.4260	residue LIG LIG LIG LIG LIG LIG LIG LIG 20e-01 2 20e-01 2 20e-01 2 20e-01 2	e atom C H H1 H2 0 H3 2.8108e 2.8108e 2.8108e 2.8108e 2.8108e 2.8108e 2.8108e	Meth: cgn: +05 +05 +05 +05 +05	r chi 1 0.22 2 0.0 3 0.0 4 0.0 5 -0.6 5 0.4	arge 049 189 189 903 287	mas 12.000000 1.000000 1.000000 1.000000 1.0000000	rges, wat	er) chargeB		
<pre>end [molecul ; Name Methanol [atoms] ; nr</pre>	Letype t aj fu aj fu aj fu 6 5 6 6 6] ype c3 h1 h1 h1 h1 h0 h0 nct 1 1 1 1 1 nct	nrexcl 3 resnr 1 1 1 1 1 1 1 1 093(1.093(1.093(1.093(9.740(1.426()))	residue LIG LIG LIG LIG LIG LIG LIG De-01 2 De-01 2 De-02 3 De-01 2	e atom C H1 H2 0 H3 2.8108e= 2.8108e= 2.8108e= 2.8108e= 2.8108e= 2.6284e=	Metha cgn: +05 +05 +05 +05 +05	r ch 1 0.2 2 0.0 3 0.0 4 0.0 5 -0.6 6 0.4	arge 049 189 189 903 287	mas 12.000000 1.000000 1.000000 1.000000 1.000000	rges, wat	er) chargeB		
<pre>end [molecul ; Name Methanol [atoms] ; nr</pre>	Letype t aj fu aj fu aj fu 6 6 6] aj 1 1 1 1 1 1] ype3 hh11 h10 h0 nct 1 1 1 1 nct ak6 3 4 5 4 5 5	nrexcl 3 resnr 1 1 1 1 1 1 1 1 093(1.093(1.093(9.7400(1.426(1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	residue LIG LIG LIG LIG LIG LIG LIG LIG LIG LIG	cth 2.8108e+ 2.81028e+ 2.8108e+ 2.8108e+ 2.81028e+ 2.8108e+	Metha cgn: +05 +05 +05 +05 +05 +05 +05 +05 +05 +05	+02 +02 +02 +02 +02 +02 +02 +02 +02 +02	arge 049 189 189 903 287	mas 12.000000 1.000000 1.000000 1.000000 1.000000	rges, wat	er) chargeB		
<pre>end [molecul ; Name Methanol [atoms] ; nr</pre>	Letype aj fu aj fu aj fu aj fu 6 6 1 1 1 1 1 1 1 1 1 1 1 1 1	$ \begin{array}{c} y \text{pe}_{\text{c}31} \\ hh1 \\ hoho \\ nct \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ $	nrexcl 3 resnr 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	residue LIG LIG LIG LIG LIG LIG LIG LIG LIG LIG	cth ++02	Metha cgn: +05 +05 +05 +05 +05 +05 +05 +05 +05 +05	+02 +02 +02 +02 +02 +02 +02 +02 +02 +02	arge 049 189 189 903 287	mas 12.000000 1.000000 1.000000 1.000000 1.000000	s typeB	er) chargeB		

end							
	Methanol	(polarize	d charges,	hexadeca	ne)		
[moleculetype] ;Name nrexcl Methanol 3							
$\begin{bmatrix} \text{atoms} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	esidue atom cgnr LIG C 1 LIG H 2 LIG H1 3 LIG H2 4 LIG 0 5 LIG H3 6	charge 0.1780 0.0193 0.0193 0.0193 -0.6357 0.3998	mass 12.000000 1.000000 1.000000 1.000000 1.000000 1.000000	typeB c	chargeB		
[bonds] ; ai aj funct r k 1 2 1 1.0930e 1 3 1 1.0930e 1 4 1 1.0930e 5 6 1 9.7400e 1 5 1 1.4260e	-01 2.8108e+05 -01 2.8108e+05 -01 2.8108e+05 -02 3.0928e+05 -01 2.6284e+05						
$\begin{bmatrix} pairs \\ ai \\ 2 \\ 6 \\ 1 \\ 3 \\ 4 \\ 6 \\ 1 \end{bmatrix}$							
$\begin{bmatrix} angles \\ ; ai \\ 1 \\ 5 \\ 6 \\ 1 \\ 2 \\ 1 \\ 3 \\ 1 \\ 2 \\ 1 \\ 4 \\ 1 \\ 3 \\ 1 \\ 4 \\ 1 \\ 5 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	heta cth .0816e+02 3.9405e+02 .0955e+02 3.2786e+02 .0955e+02 3.2786e+02 .0988e+02 4.2652e+02 .0988e+02 4.2652e+02 .0988e+02 4.2652e+02	2 2 2 2 2 2 2 2 2					
[dihedrals] ;i j k l func C 2 1 5 6 3 1 5 6 4 1 5 6	0 C5 3 0.69873 2.0 3 0.69873 2.0 3 0.69873 2.0	09618 (09618 (09618 ().00000 -).00000 -).00000 -	2.79491 2.79491 2.79491	0.00000 0.00000 0.00000	0.00000 0.00000 0.00000	; ;

1. Gromacs topologies

1,3,5 trichlorobenzene

135trichlor	obenzene	•			
12 10 10 10 10 10 10 10 10 10 10	C1 H2 C3 C4 H5 C6 C7 H8 C9 X10 1 X11 X12 1 -0.19	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 0.088\\ 0.156\\ -0.049\\ -0.138\\ -0.245\\ -0.087\\ 0.050\\ 0.089\\ 0.136\\ 0.308\\ -0.197\\ -0.112\\ 00000\\ \end{array}$	$\begin{array}{c} 0.000\\ 0.000\\ 0.000\\ -0.000\\ -0.000\\ 0.000\\ 0.000\\ -0.000\\ -0.000\\ -0.000\\ -0.000\\ -0.000\\ -0.000\\ -0.000\\ \end{array}$	
end					Chlorobenzene
Chlorobenze	ne				
12 1LIG 1LIG	C H C1	1 0.018 2 -0.037	-0.120	-0.000	
1LIG 1LIG 1LIG	H1 C2	$ \begin{array}{cccc} $	-0.120 -0.214 0.000	0.000	
1LIG 1LIG	H2 C3	6 0.335 7 0.157	-0.000 0.120	-0.000	
1LIG 1LIG	H3 C4	8 0.211 9 0.018	0.214	-0.000	
	C5 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	-0.000	-0.000	
10 05020	10 0000		0	0.000	
10.05020	10.0000	10.0000			
end					Chloroform
end					Chloroform
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000	C H CL Cl1 Cl2 1.0000	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 0 1.0000	0.000 -0.000 0.151 -0.144 -0.007	0.046 0.155 -0.009 -0.009 -0.009	Chloroform
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000 end	C H CL Cl1 Cl2 1.0000	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 0 1.0000	0.000 -0.000 0.151 -0.144 -0.007	0.046 0.155 -0.009 -0.009 -0.009	Chloroform
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000 end	CL CL CL CL CL CL CL CL CL CL CL CL CL C	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 00 1.0000	0.000 -0.000 0.151 -0.144 -0.007 00	0.046 0.155 -0.009 -0.009 -0.009	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000 end 245trichlor 14	C H CL Cl1 Cl2 1.0000	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 0 1.0000	0.000 -0.000 0.151 -0.144 -0.007	0.046 0.155 -0.009 -0.009 -0.009	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000 end 245trichlor 14 1LIG 1LIG	C H CL Cl1 Cl2 1.0000 oaniline C C1	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 00 1.0000	0.000 -0.000 0.151 -0.144 -0.007 00 -0.071 -0.119	0.046 0.155 -0.009 -0.009 -0.009	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000 end 245trichlor 14 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000	CL CL CL CL CL CL CL CL CL CL CL CL CL C	1 0.000 2 -0.000 3 0.079 5 -0.170 0 1.0000 	0.000 -0.000 0.151 -0.144 -0.007 00 -0.071 -0.119 -0.226 -0.032 0.100	0.046 0.155 -0.009 -0.009 -0.009 -0.009	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000 end 245trichlor 14 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1.00000	C H CL Cl1 Cl2 1.0000 oaniline C C C H H C2 C3 C4 H1	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 1 0.088 2 -0.042 3 -0.060 4 -0.150 5 -0.132 6 0.001	0.000 -0.000 0.151 -0.144 -0.007 00 	0.046 0.155 -0.009 -0.009 -0.009 -0.009 -0.009 0.000 0.000 0.000 0.000 0.000 -0.000	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG	C H CL Cl1 Cl2 1.0000 oaniline C C1 H C2 C3 C4 H1 C5 CCL	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 1 0.088 2 -0.042 3 -0.060 4 -0.150 5 -0.132 6 0.001 7 0.020 8 0.109 9 0.221	0.000 -0.000 0.151 -0.144 -0.007 00 -0.071 -0.119 -0.226 -0.032 0.108 0.155 0.261 0.067 -0.185	0.046 0.155 -0.009 -0.009 -0.009 -0.009 -0.009 -0.000 0.000 0.000 -0.000 -0.000 -0.000 -0.000 -0.000	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LI	C H CL Cl1 Cl2 1.0000 oaniline C C1 H C2 C3 C4 H1 C5 CL CL C1 1 1 0 0 0 1 1 0 0 0 0 0 0 1 1 0 0 0 0	1 0.000 2 -0.000 3 0.079 5 -0.170 0 1.0000 	0.000 -0.000 0.151 -0.144 -0.007 00 -0.071 -0.149 -0.226 -0.032 0.108 0.155 0.261 0.067 -0.185 0.261 0.067 -0.185 0.135 -0.097	0.046 0.155 -0.009 -0.009 -0.009 -0.000 0.000 0.000 0.000 -0.000 0.000 -0.000 0.000 -0.000 0.000 0.000 0.000 0.000 0.000 0.000	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG	C H CL Cl1 Cl2 1.0000 oaniline C C C H H C2 C3 C4 H1 C5 CL C1 1 C2 C3 C4 H1 C12 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 1 0.088 2 -0.042 3 -0.060 4 -0.150 5 -0.132 6 0.001 7 0.020 8 0.109 9 0.221 0 0.270 0 0.270 0 0.271 0 0.273 2 -0.238 3 -0.332 2 -0.223 -0.238 -0.223 -0.238 -0.223	0.000 -0.000 0.151 -0.144 -0.007 00 	0.046 0.155 -0.009 -0.009 -0.009 -0.009 -0.000 0.000 -0.000 -0.000 -0.000 -0.000 -0.000 -0.000 -0.000 -0.000 0.000 -0.000 0.000 -0.000 0.000	Chloroform 2,4,5 trichloroaniline
chloroform 5 1LIG 1LI	C H CL CL1 CL2 1.0000 0aniline C C1 H C2 C3 C4 H1 C12 C3 C4 H1 C12 C3 C4 H1 C12 C3 C4 H1 H2 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	1 0.000 2 -0.000 3 0.079 4 0.091 5 -0.170 1 0.088 2 -0.042 3 -0.060 4 -0.150 5 -0.132 6 0.001 7 0.020 8 0.109 9 0.221 0 0.270 1 -0.313 2 -0.238 3 -0.332 4 -0.223 3040 0.0	0.000 -0.000 0.151 -0.144 -0.007 00 -0.007 -0.119 -0.226 -0.032 0.108 0.155 0.261 0.067 -0.135 0.135 0.135 0.135 0.135 0.135 0.135 0.195 0.160 0.294 00000	0.046 0.155 -0.009 -0.009 -0.009 -0.009 -0.000 0.000 0.000 -0.000 0.000 -0.000 0.000 -0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	Chloroform 2,4,5 trichloroaniline

Lidocaine										
Lidocaine 39 1LIG 1LI	$ \begin{array}{ccccc} C & 1 \\ H & 2 \\ C1 & 3 \\ H1 & 4 \\ C2 & 5 \\ H2 & 6 \\ C3 & 7 \\ C4 & 8 \\ C5 & 9 \\ C6 & 10 \\ H3 & 11 \\ H4 & 12 \\ H5 & 13 \\ C7 & 14 \\ H6 & 15 \\ H7 & 16 \\ H8 & 17 \\ N & 18 \\ H9 & 19 \\ 19 \\ 19 \\ 19 \\ 22 \\ H10 & 23 \\ H11 & 24 \\ N1 & 25 \\ C10 & 26 \\ C9 & 22 \\ H10 & 23 \\ H11 & 24 \\ N1 & 25 \\ C10 & 26 \\ H12 & 27 \\ H13 & 28 \\ C11 & 29 \\ H14 & 30 \\ H15 & 31 \\ H16 & 32 \\ C12 & 33 \\ H17 & 34 \\ H18 & 35 \\ C13 & 37 \\ H19 & 37 \\ \end{array} $	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} -0.055\\ -0.052\\ -0.170\\ -0.255\\ -0.170\\ -0.263\\ -0.065\\ 0.049\\ 0.178\\ 0.269\\ 0.178\\ 0.269\\ 0.178\\ 0.269\\ 0.178\\ -0.073\\ -0.002\\ -0.073\\ -0.002\\ -0.0128\\ 0.160\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.220\\ 0.101\\ 0.003\\ 0.082\\ -0.111\\ -0.267\\ 0.008\\ 0.043\\ 0.089\\ -0.115\\ 0.0155\\ 0.015\\ 0.015\\ 0.015\\ 0.015\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.003\\ 0.015\\ 0.015\\ 0.015\\ 0.003\\$	$\begin{array}{c} -0.069\\ -0.149\\ 0.008\\ -0.011\\ 0.171\\ -0.085\\ -0.046\\ -0.131\\ -0.055\\ -0.046\\ -0.131\\ -0.071\\ -0.208\\ -0.131\\ 0.247\\ -0.208\\ -0.121\\ -0.247\\ -0.153\\ -0.052\\ -0.097\\ -0.153\\ -0.051\\ -0.051\\ -0.051\\ -0.159\\ -0.159\\ -0.159\\ -0.159\\ -0.159\\ -0.159\\ -0.159\\ -0.159\\ -0.159\\ -0.224\\ -0.121\\ -0.121\\ -0.121\\ -0.198\\ -0.110\\ -0.252\\ -0.264\\ -0.13\\ -0.062\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.086\\ -0.090\\ -0.557\\ -0.055\\ -0.086\\ -0.090\\ -0.557\\ -0.055\\ -0.$	0.0012 0.0013 0.0008 0.0005 0.0001 0.0003 0.0002 0.0002 0.0008 0.0002 0.0008 0.0002 0.0008 0.0002 0.0008 0.0002 0.0008 0.0005 0.0003 0.0005 0.0005 0.0005 0.0005 0.0005 0.0001 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	$\begin{array}{c} -0.0007\\ 0.0001\\ -0.0008\\ -0.0011\\ -0.0016\\ -0.0016\\ -0.0016\\ 0.0003\\ 0.0015\\ 0.0007\\ 0.0000\\ -0.0000\\ -0.0001\\ 0.0005\\ -0.0008\\ -0.0002\\ 0.0017\\ 0.0015\\ 0.0002\\ 0.0001\\ -0.0008\\ -0.0004\\ -0.0001\\ -0.0001\\ -0.0000\\ -0.0001\\ -0.0000\\ -0.0000\\ 0.0001\\ -0.0000\\ 0.0001\\ -0.0000\\ 0.0001\\ -0.0000\\ 0.0001\\ -0.0000\\ 0.0001\\ -0.0000\\ -0.000\\ -0.$	$\begin{array}{c} -0.0009\\ -0.0014\\ -0.0002\\ 0.0004\\ 0.0011\\ 0.0009\\ 0.0000\\ 0.0000\\ -0.0011\\ -0.0010\\ 0.0005\\ -0.0004\\ 0.0013\\ 0.0003\\ -0.0003\\ -0.0003\\ -0.0003\\ -0.0003\\ -0.0003\\ -0.0003\\ -0.0003\\ -0.0003\\ -0.0004\\ 0.0003\\ -0.0004\\ 0.0003\\ -0.0004\\ 0.0003\\ -0.0004\\ 0.0003\\ -0.0004\\ 0.0003\\ -0.0000\\ -0.000\\ -$			
	H19 37 H20 38	-0.298 -	-0.155 -0.188	0.157 0.023 - 0.151 -	0.0000	-0.0000	-0.0000			
2.50890	2.02520	2.10950	-0.011	0.151 -	0.0000	0.0000	0.0000			
end						·		 	 	
Mathenal						Metha	nol			
6 1LIG 1LIG 1LIG 1LIG 1LIG 1LIG 0.57520	C 1 H 2 H1 3 H2 4 0 5 H3 6 0.51230	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-0.003 -0.058 -0.055 0.097 0.009 -0.081	-0.000 -0.088 0.090 -0.001 -0.003 -0.002						

end-----

Lidocaine