

\*stream file for R1 parameters  
\*stream after the charmm param27 file  
\*

read param card append  
\* SLX  
\*

BONDS

NN	ON	485.17	1.264	!	H	R	T	P	1
NN	CTL1	182.65	1.444	!	H	R	T	P	1
CEL1	CTL1	240.00	1.502	!					

ANGLES

CTL1	NN	ON	45.12	115.52	!	H	R	T	P	1
CTL1	NN	CTL1	38.60	119.08	!	H	R	T	P	1
NN	CTL1	CTL3	51.55	104.19	!	H	R	T	P	3
NN	CTL1	CTL2	51.55	104.19	!	-	-	-	-	0
NN	CTL1	CTL1	51.55	104.19	!	-	-	-	-	0
NN	CTL1	CEL1	64.23	103.75	!	X	X	X	P	1
CTL1	CEL1	CTL2	45.15	112.75	!	X	X	X	P	2
CTL1	CEL1	CTL3	45.15	112.75	!	-	-	-	-	0
HEL1	CEL1	CTL1	30.66	103.41	!	X	X	X	P	1
CTL3	CTL1	CEL1	32.49	112.20	!					
CEL1	CEL1	CTL1	48.00	123.50	!					
!										
!	CTL2	CTL1	CTL2	58.350	113.50	11.16	2.561	!	glycerol	
CTL3	CTL1	CTL3	58.350	113.50	11.16	2.561	!	glycerol		
!link										
SM	CTL2	CEL1	58.000	112.5000	!	ALLOW	ALI	SUL	ION	
CTL3	CEL1	CTL2	42.63	112.34	!	X	X	X	P	2
!										
!compare										
!	HEL1	CEL1	CTL2	40.00	116.00	!	from	propene,	yin,adm	jr., 12/95
!	HEL1	CEL1	CTL3	22.00	117.00	!	propene,	yin,adm	jr., 12/95	

DIHEDRALS

ON	NN	CTL1	CTL3	0.099	3	0.00	!	H	R	T	P	3
ON	NN	CTL1	CTL2	0.099	3	0.00	!	-	-	-	-	0
ON	NN	CTL1	CTL1	0.099	3	0.00	!	-	-	-	-	0
ON	NN	CTL1	CEL1	0.052	3	0.00	!	X	X	X	P	1
HAL3	CTL3	CTL1	NN	0.093	3	0.00	!	H	R	T	P	2
HAL2	CTL2	CTL1	NN	0.093	3	0.00	!	-	-	-	-	0
NN	CTL1	CTL1	CTL2	0.481	3	0.00	!	X	R	X	X	2
NN	CTL1	CTL1	CTL3	0.481	3	0.00	!	-	-	-	-	0
CTL3	CTL1	CTL2	CTL2	0.151	3	0.00	!	H	R	X	X	2
CTL3	CTL1	CTL2	CTL1	0.151	3	0.00	!	-	-	-	-	0
HAL3	CTL3	CTL1	CTL2	0.046	3	0.00	!	H	R	T	X	2
HAL3	CTL3	CTL1	CTL1	0.046	3	0.00	!	-	-	-	-	0
NN	CTL1	CTL2	CTL2	0.593	3	0.00	!	H	R	X	X	2
NN	CTL1	CTL2	CTL1	0.593	3	0.00	!	-	-	-	-	0
CTL1	CTL1	CTL2	CTL1	1.368	3	0.00	!	X	R	X	X	1
CTL3	CTL1	CTL1	CTL2	0.104	3	0.00	!	X	R	X	X	2
CTL3	CTL1	CTL1	CTL3	0.104	3	0.00	!	-	-	-	-	0
NN	CTL1	CEL1	CEL1	3.178	3	0.00	!	X	X	X	P	1
NN	CTL1	CEL1	CTL3	-0.312	3	0.00	!	X	X	X	P	2
NN	CTL1	CEL1	CTL2	-0.312	3	0.00	!	-	-	-	-	0

NN	CTL1	CEL1	HEL1	2.165	3	0.00	!	X	X	X	P	1
CTL3	CEL1	CTL1	CTL3	0.308	3	0.00	!	X	X	X	P	2
CTL2	CEL1	CTL1	CTL3	0.308	3	0.00	!	-	-	-	-	0
CEL1	CEL1	CTL1	CTL3	0.500	1	180.00	!					
CEL1	CEL1	CTL1	CTL3	1.300	3	180.00	!					
!CTL1	CEL1	CEL1	CTL1	0.226	2	0.00	!	X	X	X	P	1
!CTL1	CEL1	CEL1	CTL2	0.247	2	180.00	!	X	X	X	P	2
!CTL1	CEL1	CEL1	CTL3	0.247	2	180.00	!	-	-	-	-	0
!use												
!X	CEL1	CEL1	X	0.1500	1	0.00	!	2-butene, adm jr., 2/00 update				
!X	CEL1	CEL1	X	8.5000	2	180.00	!	2-butene, adm jr., 2/00 update				
!zeros												
CTL1	NN	CTL1	CTL3	0.0	3	0.00	!	H	R	T	P	2
CTL1	NN	CTL1	CTL2	0.0	3	0.00	!	-	-	-	-	0
CTL1	NN	CTL1	CTL1	0.0	3	0.00	!	X	R	X	X	1
CTL1	NN	CTL1	CEL1	0.0	3	0.00	!	X	X	X	P	1
HAL3	CTL3	CTL1	CEL1	0.0	3	0.00	!	X	X	X	P	1
!HAL2	CTL2	CEL1	CTL1	0.617	3	0.00	!	X	X	X	P	1
!compare from cholest												
!HAL3	CTL3	CEL1	CTL1	0.0300	3	0.0	!	HAL2	CTL2	CEL1	CTL1	0.03 3 0.0
!												
!link												
!HAL3	CTL3	CEL1	CTL1	0.090	3	0.00	!	X	X	X	P	X 1
!SCAN-DIHEDRALS												
SM	CTL2	CEL1	CEL1	-0.274	1	0.00	!	X	X	X	P	X 1
SM	CTL2	CEL1	CEL1	0.220	2	0.00	!	X	X	X	P	X 1
SM	CTL2	CEL1	CEL1	-0.105	3	0.00	!	X	X	X	P	X 1
SM	CTL2	CEL1	CTL1	0.145	1	0.00	!	X	X	X	P	X 1
SM	CTL2	CEL1	CTL1	-0.049	2	0.00	!	X	X	X	P	X 1
SM	CTL2	CEL1	CTL1	0.048	3	0.00	!	X	X	X	P	X 1
HAL2	CTL2	CEL1	CTL1	-0.029	1	0.00	!	X	X	X	P	X 1
HAL2	CTL2	CEL1	CTL1	0.135	2	0.00	!	X	X	X	P	X 1
HAL2	CTL2	CEL1	CTL1	0.000	3	0.00	!	X	X	X	P	X 1
SM	SM	CTL2	CEL1	0.063	3	0.00	!	X	X	X	P	X 1
SM	CT2	CT1	NH1	-0.066	1	0.00	!	X	X	X	X	A 1
SM	CT2	CT1	NH1	0.053	2	0.00	!	X	X	X	X	A 1
SM	CT2	CT1	NH1	0.237	3	0.00	!	X	X	X	X	A 1
SM	CT2	CT1	C	0.233	1	0.00	!	X	X	X	X	A 1
SM	CT2	CT1	C	-0.005	2	0.00	!	X	X	X	X	A 1
SM	CT2	CT1	C	0.149	3	0.00	!	X	X	X	X	A 1
SM	CTL2	CTL1	HAL1	0.064	3	0.00	!	X	R	X	X	A 2
SM	CT2	CT1	HB	0.064	3	0.00	!	-	-	-	-	0
!dih2-dih4												
!SM	SM	CT2	CT1	0.31	3	0.00	!	X	R	X	X	A 2
!SM	SM	CTL2	CTL1	0.31	3	0.00	!	-	-	-	-	0
! do not change												
!SM	SM	CT2	HA	0.1580	3	0.00	!	X	X	X	X	A 1
!SM	SM	CTL2	HAL2	0.1580	3	0.00	!	-	-	-	-	0

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!uses
!X   CTL1 CTL2 X       0.200  3   0.00 ! alkane, 3/92
!HAL2 CTL2 CEL1 CTL1   0.000  3   0.00 ! X X X P 1 (OK to use cholesterol)
!
HAL2 CTL2 CTL1 CTL3    0.1200  3   0.00 ! lkr5 dih5
!
!THIS HAS TO BE DONE AND : HAL3 CTL3 CEL1 CTL1    0.0600  3  0.0
!LARGER THAN THE EXISTING: HAL2 CTL2 CEL1 CTL1    0.0300  3  0.0
!POTENTIAL PROBLEM!!!
!
!
!take
!CTL3 CEL1 CEL1 HEL1    1.0000  2  180.00 ! 2-butene, adm jr., 8/98 update
CTL2 CEL1 CEL1 HEL1    1.0000  2  180.00 ! " "
CTL1 CEL1 CEL1 HEL1    1.0000  2  180.00 ! " "
!CTL2 CEL1 CTL1 CTL3    0.00    3  180.0  ! br12
!
!compare
!HEL1 CEL1 CTL2 CTL2    0.1200  3   0.00 ! butene, yin,adm jr., 12/95
!HEL1 CEL1 CTL2 CTL3    0.1200  3   0.00 ! butene, yin,adm jr., 12/95
HEL1 CEL1 CTL1 CTL3    0.1200  3   0.00 ! butene, yin,adm jr., 12/95
!

IMPROPER
CTL1 CEL1 CEL1 CTL3    4.193  0  180.00 ! X X X P 2
CTL1 CEL1 CEL1 CTL2    4.193  0  180.00 ! - - - - 0
CTL1 CEL1 CEL1 HEL1    9.878  0  180.00 ! X X X P 1

NONBONDED
!nitroxide
NN      0.0      -0.20      1.85  ! as all other nitogens
ON      0.0      -0.1521     1.77
ONr     0.0      -0.1521     1.77

END

return

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