```
*stream file for R1 topology
*to be treamed after the charmm topology file
*

read rtf card append
* ////////// \\\\\\\\\ July 4th 2006 /////////\\\\\\\\\
*
27 1

MASS 200  ON   15.999400 O ! spin label O
MASS 201  NN   14.007000 O ! spin label N

DEFA FIRS none LAST none
AUTOGENERATE ANGLES DIHEDRALS

RESI R1          0.00 ! Spin Label for Proteins       chi2(pot) = 0.03406
GROUP                 !
ATOM O    ON    -0.438!              H1A
ATOM N    NN     0.220!      H1B\   /
ATOM C1   CTL1   0.334!          C1A
ATOM C2   CTL1   0.329!          |  \H1C
GROUP
ATOM C1A  CTL3  -0.337!          |                    H2A
ATOM H1A  HAL3   0.09 !          |            H2B\   /
ATOM H1B  HAL3   0.09 !          |                C2A
ATOM H1C  HAL3   0.09 !          |               /   \H2C
GROUP                 !                 O
ATOM C2A  CTL3  -0.335!          |       |      /
ATOM H2A  HAL3   0.09 !           \      N     /
ATOM H2B  HAL3   0.09 !            \  /   \  /
ATOM H2C  HAL3   0.09 !              C1     C2 ----
GROUP
ATOM C1D  CTL3  -0.337!           /  |     |       \
ATOM H1D  HAL3   0.09 !          /  C1R===C2R-H2R   \
ATOM H1E  HAL3   0.09 !          |   |                |
ATOM H1F  HAL3   0.09 !
GROUP
ATOM C2D  CTL3  -0.335!          |   |               | /H2D
ATOM H2D  HAL3   0.09 !          |    \             C2D
ATOM H2E  HAL3   0.09 !          |     \       H2E/   \
ATOM H2F  HAL3   0.09 !          |      |               H2F
GROUP
ATOM C1R  CEL1  -0.003!     H1D\ |      |
ATOM C2R  CEL1  -0.340!         C1D     |
ATOM H2R  HEL1   0.162!        /  \H1E  |
GROUP                 !      H1F       |
ATOM C1L  CTL2  -0.10 !               - C1L -
ATOM H1L  HAL2   0.09 !                  |
ATOM H1M  HAL2   0.09 !                  |
ATOM S1L  SM    -0.08 !                S1L
GROUP                 !                 |
ATOM S2L  SM    -0.08 !                S2L
ATOM C2L  CTL3  -0.19 !                 |
ATOM H2L  HAL3   0.09 !                C2L
ATOM H2M  HAL3   0.09 !               / | \
ATOM H2N  HAL3   0.09 !            H2L H2M H2N
DOUBLE  C1R  C2R
```

```
BOND  O    N
BOND  N    C1        N    C2
BOND  C1A  C1        C1D  C1
BOND  C2A  C2        C2D  C2
BOND  H1A  C1A       H1B  C1A       H1C  C1A
BOND  H1D  C1D       H1E  C1D       H1F  C1D
BOND  H2A  C2A       H2B  C2A       H2C  C2A
BOND  H2D  C2D       H2E  C2D       H2F  C2D
BOND  C1   C1R       C2   C2R       H2R  C2R
BOND  C1L  C1R
BOND  H1L  C1L       H1M  C1L       C1L  S1L
BOND  S1L  S2L       S2L  C2L
BOND  C2L  H2L       C2L  H2M       C2L  H2N
IMPR  C2  C1R  C2R  H2R
IMPR  C1  C2R  C1R  C1L
CMAP  C2R  C1R  C1L  S1L    C1R  C1L  S1L  S2L
ACCEPTOR O N
IC      C1R   C1    N     C2     1.5278   98.53   -1.45  116.77   1.4647
IC      C1    N     C2    C2R    1.4662  116.77    1.60   99.75   1.5086
IC      N     C2    C2R   C1R    1.4647   99.75   -1.06  112.12   1.3357
IC      C2    C2R   C1R   C1     1.5086  112.12    0.26  112.81   1.5278
IC      C2R   C1R   C1    N      1.3357  112.81    0.67   98.53   1.4662
IC      C1R   C1    N     O      1.5278   98.53  178.95  121.79   1.2905
IC      C2R   C1R   C1    C1A    1.3357  112.81 -115.07  114.52   1.5406
IC      C2R   C1R   C1    C1D    1.3357  112.81  115.60  112.69   1.5415
IC      C2A   C2    C2R   C1R    1.5369  111.79  115.05  112.12   1.3357
IC      C2D   C2    C2R   C1R    1.5373  111.69 -117.01  112.12   1.3357
IC      C1L   C1R   C1    N      1.5092  121.37 -178.90   98.53   1.4662
IC      C1L   C1R   C2R   C2     1.5092  125.82  179.81  112.12   1.5086
IC      C1    C1R   C1L   S1L    1.5088  116.75   79.83  108.84   1.8702
IC      C2R   C1R   C1L   S1L    1.3382  120.56  -99.58  108.84   1.8702
IC      C1R   C1L   S1L   S2L    1.5078  108.84 -164.49  103.76   2.0813
IC      C1L   S1L   S2L   C2L    1.8702  103.76   88.88  103.36   1.8366


PRES LKR1        -0.36 ! Patch must be 1-CYS and 2-R1.
GROUP                  ! use in a patch statement
ATOM 1CB   CT2   -0.10 !                    |
ATOM 1SG   SM    -0.08 !           2S1L--2C1L--
GROUP                  !   |      /        |
ATOM 2S1L  SM    -0.08 ! -1CB--1SG
ATOM 2C1L  CTL2  -0.10 !   |
DELETE ATOM 1HG1
DELETE ATOM 2S2L
DELETE ATOM 2C2L
DELETE ATOM 2H2L
DELETE ATOM 2H2M
DELETE ATOM 2H2N
BOND 1SG 2S1L
ANGLE 1CB  1SG   2S1L            1SG   2S1L  2C1L
DIHE 1HB1  1CB   1SG   2S1L      1HB2  1CB   1SG   2S1L
DIHE 2H1L  2C1L  2S1L  1SG       2H1M  2C1L  2S1L  1SG
DIHE 1CA   1CB   1SG   2S1L      1SG   2S1L  2C1L  2C1R
DIHE 1SG   2S1L  2C1L  2H1L      1SG   2S1L  2C1L  2H1M
DIHE 1CB   1SG   2S1L  2C1L
CMAP 2C2R  2C1R  2C1L  2S1L      2C1R  2C1L  2S1L  1SG
IC 1CA  1CB   1SG   2S1L  0.0000  0.0000  180.0000  0.0000  0.0000
```

```
IC 1CB  1SG   2S1L  2C1L  0.0000  0.0000   90.0000  0.0000  0.0000
IC 1SG  2S1L  2C1L  2C1R  0.0000  0.0000  180.0000  0.0000  0.0000


END
```

```
*stream file for R1 parameters
*stram 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
```

```
!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
```

```
*stream file for R1 cmap parameters
*

read param card append
* SLX
*

CMAP

CEL1 CEL1 CTL2 SM    CEL1 CTL2 SM   SM    12
!r1 cmap
! -180.0
  2.358500  2.399450  2.438250  1.477750  0.316250
 -1.122600 -2.924300 -1.122600  0.316250  1.477750
  2.438250  2.399450

! -150.0
  0.400750  0.661800  0.651400  0.379950 -1.587150
 -3.304950 -2.133000 -0.907000 -0.796800  0.320100
  0.819950  0.793850

! -120.0
 -0.429400 -0.103400 -0.023200 -1.043250 -2.155050
 -0.983100 -0.486950 -0.866250 -0.524550 -0.272550
 -0.068900 -0.269050

!  -90.0
 -0.011300  0.192750  0.118500  0.307850  1.454700
  1.297300  0.421000  0.122450 -0.068200  0.437750
  0.848100  0.480250

!  -60.0
  0.006650  0.732450  1.608600  1.970050  1.863050
  1.261600  0.627600  0.582650  0.923650  1.437400
  1.476100  0.615100

!  -30.0
 -0.286950  0.507900  0.767750  0.459850 -0.070250
  0.026850 -0.117250 -0.187200  0.170750 -0.091200
 -0.181850 -0.508950

!    0.0
 -0.514300 -0.564250 -0.766600 -0.930950 -0.936500
 -0.692050 -1.160300 -0.692050 -0.936500 -0.930950
 -0.766600 -0.564250

!   30.0
 -0.286950 -0.508950 -0.181850 -0.091200  0.170750
 -0.187200 -0.117250  0.026850 -0.070250  0.459850
  0.767750  0.507900

!   60.0
  0.006650  0.615100  1.476100  1.437400  0.923650
  0.582650  0.627600  1.261600  1.863050  1.970050
  1.608600  0.732450

!   90.0
```

```
 -0.011300  0.480250  0.848100  0.437750 -0.068200
  0.122450  0.421000  1.297300  1.454700  0.307850
  0.118500  0.192750

!  120.0
 -0.429400 -0.269050 -0.068900 -0.272550 -0.524550
 -0.866250 -0.486950 -0.983100 -2.155050 -1.043250
 -0.023200 -0.103400

!  150.0
  0.400750  0.793850  0.819950  0.320100 -0.796950
 -0.906950 -2.133000 -3.304950 -1.587400  0.379950
  0.651400  0.661800


CTL1 CTL1 CTL2 SM    CTL1 CTL2 SM   SM    12
!r5 cmap
! -180.0
  0.326800  0.391900  0.132600 -0.193900  0.075000
 -0.515500 -0.494900 -0.096900  0.208500 -0.183100
 -0.255800 -0.005250

! -150.0
  0.532400  0.258000  0.183950  0.129100  0.653450
  0.788250  0.513950  0.462900  0.790600  0.723300
  0.595500  0.694250

! -120.0
  0.100900  0.070800  0.141250  0.406150  0.593450
  0.148150 -0.714950  0.583800  1.085000  0.296350
  0.168600  0.379850

!  -90.0
  0.237600  0.157050  0.110000  0.350000  0.418000
 -0.221450 -0.020400 -1.108650 -1.661750 -0.574950
  0.480900  0.490550

!  -60.0
  0.483850  0.080550 -0.067550  0.222400  0.064450
 -0.287100 -2.273750 -2.890150 -1.485950  0.136050
  1.013300  0.990850

!  -30.0
  1.056500  0.455350  0.092550  0.039750 -0.446100
 -2.239400 -3.664400 -3.188950 -1.461150 -0.010350
  0.722750  1.535150

!    0.0
  0.297900 -0.184000 -0.038100 -0.331350 -1.336800
 -3.498250 -4.944750 -4.182900 -2.311050 -0.589200
  0.795100  0.900800

!   30.0
 -0.692400  0.051650  0.229850 -0.318000 -2.264500
 -4.437150 -6.106950 -3.620550 -0.952950 -0.210300
 -0.164550 -0.669650
```

```
!   60.0
  0.232400  1.060900  0.046550 -2.025900 -3.747950
 -4.395350 -2.648550 -0.981250  0.119250 -0.528650
 -1.055200 -0.897850

!   90.0
  1.198600  1.212000  0.227300 -0.463000 -0.572750
 -1.127650 -1.412400 -0.411500  0.433250 -0.015800
  0.225650  0.794400

!  120.0
  0.897850  1.118250  0.868800  1.007050  0.159550
 -1.027750 -1.105550 -0.597100 -0.395100 -0.085550
  0.549850  0.783150

!  150.0
  0.452650  0.684650  0.624900  0.047800 -0.193350
 -0.620400 -1.803000 -1.558350 -0.718700 -0.113650
 -0.147750  0.130950


NH1 CT1 CT2 SM    CT1 CT2 SM   SM    12
!adds cmap
! -180.0
 -0.178600  0.777600  1.057250 -0.395900 -0.842300
  0.021150  1.265600 -0.100000 -0.775750  0.085900
 -0.107800 -0.379100

! -150.0
  0.631550  1.153100  0.260150 -1.022150  0.311400
  1.411000  0.320500 -0.675000  0.436250  0.521500
  0.034500  0.091000

! -120.0
 -0.308300 -0.104050 -0.937950 -1.103300  0.067650
 -0.775800 -2.071700 -0.678300 -0.131800 -0.477000
 -0.652950 -0.453050

!  -90.0
 -0.065550  0.058850 -0.334250 -0.205550 -0.059850
 -0.800200 -0.240200  0.602150 -0.150850 -0.893450
 -0.588200 -0.409900

!  -60.0
  0.796750  1.164200  0.977400  0.499900  0.161700
  0.454900  1.804950  1.677250  0.607500  0.564550
  0.608700  0.432150

!  -30.0
  2.225100  2.828000  1.720500  0.500300  0.445300
  2.132450  2.128150  1.627750  2.237900  2.292250
  1.090400  1.410050

!    0.0
  3.471450  2.416650  0.703850  0.311100  1.745250
  1.659500  0.602700  1.741500  2.339250  1.095950
  0.609700  2.165250
```

```
!   30.0
  2.649250  1.530150  0.875750  1.933150  2.308250
  1.993500  2.337700  2.267950  1.466750  0.569500
  1.635000  3.272050

!   60.0
  1.290800  0.125900  0.182300  0.730700  1.712400
  1.941250  1.323300  0.701900  0.351650  0.218850
  1.701050  2.119250

!   90.0
  0.192050 -0.050750  0.076400  0.109700 -0.132300
  0.432750  0.085050 -0.557700  0.213900 -0.003400
  0.579550  0.806950

!  120.0
 -0.564150 -0.785050 -1.166700 -1.716300 -0.868450
 -0.961350 -2.520200 -1.396600 -0.705100 -2.088800
 -1.682650 -0.922050

!  150.0
 -1.272000 -0.959300 -0.797100 -0.470400 -0.952850
 -2.219150 -1.613850 -0.195800 -2.266700 -2.141550
 -1.242500 -0.849750


END

return
```

```
*stream file for the cholesterol and SM-lipid parameters
*

read param card append
* SLX
*

BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
!
!cholesterol
!CEL1  CTL1  240.000     1.502   ! from CEL1  CTL2: sR12cc (c8-c39)
!
!disulfide
SM   CTL2  214.000     1.8160 ! ALLOW   SUL ION
               ! improved CSSC dihedral in DMDS  5/15/92 (FL)
SM   CTL3  214.000     1.8160 ! ALLOW   SUL ION
               ! improved CSSC dihedral in DMDS  5/15/92 (FL)

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
!
!cholesterol
!CTL1 CTL2 CEL1   32.00     112.20   !from CEL1 CTL2 CTL2
!CTL2 CTL1 CEL1   32.00     112.20   !from CEL1 CTL2 CTL2
!CTL1 CTL1 CEL1   32.00     112.20   !from CEL1 CTL2 CTL2
!CTL3 CTL1 CEL1   32.00     112.20   !from CEL1 CTL2 CTL2
!CTL1 CEL1 CTL2   50.00     113.00   !guess FC, eq. angle to yield 360 deg sum
!CEL1 CEL1 CTL1   48.00     123.50   ! from CEL1 CEL1 CTL2/3
!CTL3 CTL1 CTL3   53.350    108.50    8.00   2.561  ! from CTL1 CTL1 CTL3, for
IC build only
!
!disulfide
SM   CTL2 CTL1   58.000   112.5000 ! ALLOW   ALI SUL ION
               ! as in expt.MeEtS & DALC crystal,  5/15/92
SM   CTL2 HAL2   38.000   111.0000 ! ALLOW   ALI SUL ION
               ! new S-S atom type 8/24/90
SM   CTL3 HAL3   38.000   111.0000 ! ALLOW   ALI SUL ION
               ! new S-S atom type 8/24/90
SM   SM   CTL2   72.500   103.3000 ! ALLOW   ALI SUL ION
               ! expt. dimethyldisulfide,    3/26/92 (FL)
```

```
SM   SM   CTL3   72.500   103.3000 ! ALLOW   ALI SUL ION
               ! expt. dimethyldisulfide,    3/26/92 (FL)

DIHEDRALS
!
!V(dihedral) = Kchi(1  cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!
!cholesterol
!CTL1 CTL2 CEL1 CTL1     0.30    3   180.0  ! torR1
!CTL2 CEL1 CTL1 CTL1     0.00    3   180.0  ! bR12
!CTL2 CEL1 CTL1 CTL3     0.00    3   180.0  ! bR12
!CTL2 CEL1 CTL1 CTL2     0.30    3   180.0  ! torR1
!HAL2 CTL2 CEL1 CTL1     0.0300  3     0.0  ! CH2 wag and twist, from CEL1 CEL1
CTL2 HAL2
!CEL1 CEL1 CTL2 CTL1     0.5000  1   180.0  ! torR2, CEL1 CEL1 CTL2 CTL2
!CEL1 CEL1 CTL2 CTL1     1.3000  3   180.0  !
!CEL1 CEL1 CTL1 CTL1     0.5000  1   180.0  ! torR2, CEL1 CEL1 CTL2 CTL2
!CEL1 CEL1 CTL1 CTL1     1.3000  3   180.0  !
!CEL1 CEL1 CTL1 CTL2     0.5000  1   180.0  ! bR12, CEL1 CEL1 CTL2 CTL2
!CEL1 CEL1 CTL1 CTL2     1.3000  3   180.0  !
!CEL1 CEL1 CTL1 CTL3     0.5000  1   180.0  ! bR13, rCH3, CEL1 CEL1 CTL2 CTL2
!CEL1 CEL1 CTL1 CTL3     1.3000  3   180.0  !
!HEL1 CEL1 CTL2 CTL1     0.00    3     0.0  ! wC9H, HEL1 CEL1 CTL2 CTL2
!disulfide
CT2  SM   SM   CTL2     1.0000  1     0.00 ! ALLOW   ALI SUL ION
CT2  SM   SM   CTL2     4.1000  2     0.00 ! ALLOW   ALI SUL ION
CT2  SM   SM   CTL2     0.9000  3     0.00 ! ALLOW   ALI SUL ION
CT2  SM   SM   CTL3     1.0000  1     0.00 ! ALLOW   ALI SUL ION
CT2  SM   SM   CTL3     4.1000  2     0.00 ! ALLOW   ALI SUL ION
CT2  SM   SM   CTL3     0.9000  3     0.00 ! ALLOW   ALI SUL ION
CTL3 SM   SM   CTL2     1.0000  1     0.00 ! ALLOW   ALI SUL ION
CTL3 SM   SM   CTL2     4.1000  2     0.00 ! ALLOW   ALI SUL ION
CTL3 SM   SM   CTL2     0.9000  3     0.00 ! ALLOW   ALI SUL ION
SM   SM   CTL2 CTL2     0.3100  3     0.00 ! ALLOW  SUL ALI
SM   SM   CTL2 CTL1     0.3100  3     0.00 ! ALLOW  SUL ALI
SM   SM   CTL2 HAL2     0.1580  3     0.00 ! ALLOW   ALI SUL ION
SM   SM   CTL3 HAL3     0.1580  3     0.00 ! ALLOW   ALI SUL ION
SM   CTL2 CTL2 HAL2     0.0100  3     0.00 ! ALLOW   ALI SUL ION


IMPROPER
!
!V(improper) = Kpsi(psi - psi0)**2
!
!Kpsi: kcal/mole/rad**2
!psi0: degrees
!note that the second column of numbers (0) is ignored
!
!atom types           Kpsi                   psi0
!
```

```
END
```