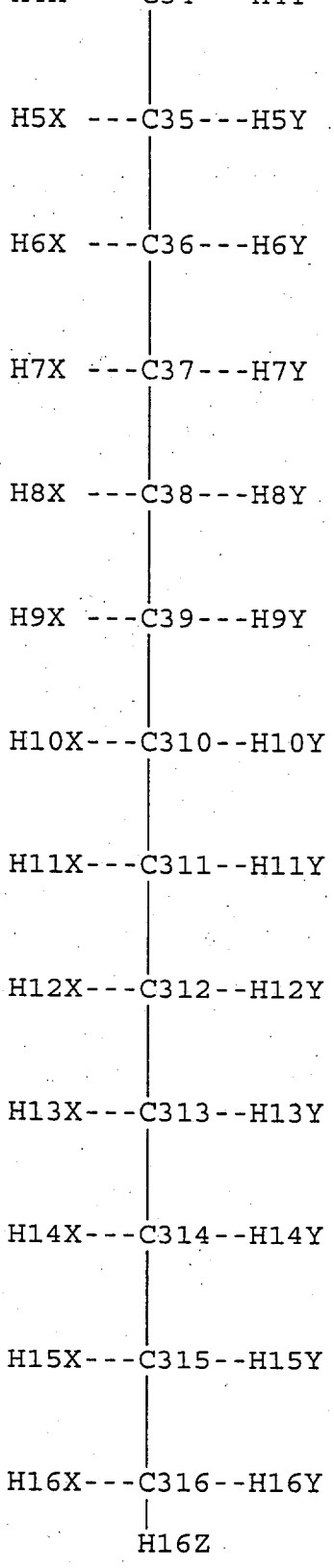
```
ATOM H4X  HAL2    0.09 !
ATOM H4Y  HAL2    0.09 !
GROUP                  !
ATOM C35  CTL2   -0.18 !
ATOM H5X  HAL2    0.09 !
ATOM H5Y  HAL2    0.09 !
GROUP                  !
ATOM C36  CTL2   -0.18 !
ATOM H6X  HAL2    0.09 !
ATOM H6Y  HAL2    0.09 !
GROUP                  !
ATOM C37  CTL2   -0.18 !
ATOM H7X  HAL2    0.09 !
ATOM H7Y  HAL2    0.09 !
GROUP                  !
ATOM C38  CTL2   -0.18 !
ATOM H8X  HAL2    0.09 !
ATOM H8Y  HAL2    0.09 !
GROUP                  !
ATOM C39  CTL2   -0.18 !
ATOM H9X  HAL2    0.09 !
ATOM H9Y  HAL2    0.09 !
GROUP                  !
ATOM C310 CTL2   -0.18 !
ATOM H10X HAL2    0.09 !
ATOM H10Y HAL2    0.09 !
GROUP                  !
ATOM C311 CTL2   -0.18 !
ATOM H11X HAL2    0.09 !
ATOM H11Y HAL2    0.09 !
GROUP                  !
ATOM C312 CTL2   -0.18 !
ATOM H12X HAL2    0.09 !
ATOM H12Y HAL2    0.09 !
GROUP                  !
ATOM C313 CTL2   -0.18 !
ATOM H13X HAL2    0.09 !
ATOM H13Y HAL2    0.09 !
GROUP                  !
ATOM C314 CTL2   -0.18 !
ATOM H14X HAL2    0.09 !
ATOM H14Y HAL2    0.09 !
GROUP                  !
ATOM C315 CTL2   -0.18 !
ATOM H15X HAL2    0.09 !
ATOM H15Y HAL2    0.09 !
GROUP                  !
ATOM C316 CTL3   -0.27 !
ATOM H16X HAL3    0.09 !
ATOM H16Y HAL3    0.09 !
ATOM H16Z HAL3    0.09 !
```




```
! Polar Head
BOND  N     HN1        N     HN2        N     HN3        N     C12
BOND  C12   H12A       C12   H12B       C12   C11
BOND  C11   H11A       C11   H11B       C11   O12
BOND  O12   P          P     O11        P     O13        P     O14
! Glycerol Backbone
BOND  C1    HA         C1    HB         C1    C2         C1    O11
BOND  C2    HS         C2    C3         C2    O21
```

```
BOND  C3   HX       C3   HY       C3   O31
! Chain from C2
BOND  O21  C21
BOND  C21  C22
DOUBLE  C21  O22
BOND  C22  H2R      C22  H2S      C22  C23
BOND  C23  H3R      C23  H3S      C23  C24
BOND  C24  H4R      C24  H4S      C24  C25
BOND  C25  H5R      C25  H5S      C25  C26
BOND  C26  H6R      C26  H6S      C26  C27
BOND  C27  H7R      C27  H7S      C27  C28
BOND  C28  H8R      C28  H8S      C28  C29
BOND  C29  H91
DOUBLE  C29 C210
BOND  C210 H101     C210 C211
BOND  C211 H11R     C211 H11S     C211 C212
BOND  C212 H12R     C212 H12S     C212 C213
BOND  C213 H13R     C213 H13S     C213 C214
BOND  C214 H14R     C214 H14S     C214 C215
BOND  C215 H15R     C215 H15S     C215 C216
BOND  C216 H16R     C216 H16S     C216 C217
BOND  C217 H17R     C217 H17S     C217 C218
BOND  C218 H18R     C218 H18S     C218 H18T
! Chain From C3
BOND  O31  C31
BOND  C31  C32
DOUBLE  C31  O32
BOND  C32  H2X      C32  H2Y      C32  C33
BOND  C33  H3X      C33  H3Y      C33  C34
BOND  C34  H4X      C34  H4Y      C34  C35
BOND  C35  H5X      C35  H5Y      C35  C36
BOND  C36  H6X      C36  H6Y      C36  C37
BOND  C37  H7X      C37  H7Y      C37  C38
BOND  C38  H8X      C38  H8Y      C38  C39
BOND  C39  H9X      C39  H9Y      C39  C310
BOND  C310 H10X     C310 H10Y     C310 C311
BOND  C311 H11X     C311 H11Y     C311 C312
BOND  C312 H12X     C312 H12Y     C312 C313
BOND  C313 H13X     C313 H13Y     C313 C314
BOND  C314 H14X     C314 H14Y     C314 C315
BOND  C315 H15X     C315 H15Y     C315 C316
BOND  C316 H16X     C316 H16Y     C316 H16Z

IMPR C21 O21 C22 O22    C31 O31 C32 O32

!IC table from IC generate, geometry is guessed
IC HN1  C12  *N   HN2  1.0524  110.54  127.93  115.12  1.0338
IC HN1  C12  *N   HN3  1.0524  110.54 -112.33  100.76  1.0488
IC HN1  N    C12  C11  1.0524  110.54   70.07  107.99  1.5341
IC C11  N    *C12 H12A 1.5341  107.99 -122.80  109.40  1.1069
IC H12A N    *C12 H12B 1.1069  109.40 -119.69  107.75  1.1114
IC N    C12  C11  O12  1.5038  107.99   46.85  109.27  1.4315
IC O12  C12  *C11 H11A 1.4315  109.27 -121.18  109.30  1.1164
IC H11A C12  *C11 H11B 1.1164  109.30 -117.51  109.07  1.1179
IC C12  C11  O12  P    1.5341  109.27  178.59  119.49  1.5904
IC C11  O12  P    O11  1.4315  119.49  104.93  100.57  1.5835
IC O11  O12  *P   O13  1.5835  100.57 -114.66  107.37  1.4782
IC O11  O12  *P   O14  1.5835  100.57  115.52  107.48  1.4694
IC O12  P    O11  C1   1.5904  100.57  -68.41  122.45  1.4279
IC P    O11  C1   C2   1.5835  122.45  113.33  109.83  1.5458
```

```
IC C2   O11  *C1  HA   1.5458 109.83  118.28 108.95  1.1134
IC HA   O11  *C1  HB   1.1134 108.95  118.31 112.84  1.1153
IC O11  C1   C2   O21  1.4279 109.83 -169.38 109.43  1.4399
IC O21  C1   *C2  C3   1.4399 109.43 -120.76 111.51  1.5508
IC C3   C1   *C2  HS   1.5508 111.51 -116.85 107.06  1.1136
IC C1   C2   O21  C21  1.5458 109.43  123.06 117.42  1.3213
IC C2   O21  C21  C22  1.4399 117.42  163.64 109.74  1.5303
IC C22  O21  *C21 O22  1.5303 109.74 -176.86 126.01  1.2239
IC O21  C21  C22  C23  1.3213 109.74 -113.72 109.53  1.5428
IC C23  C21  *C22 H2R  1.5428 109.53  120.69 110.65  1.1107
IC H2R  C21  *C22 H2S  1.1107 110.65  118.78 108.83  1.1092
IC C1   C2   C3   O31  1.5458 111.51 -171.21 111.32  1.4465
IC O31  C2   *C3  HX   1.4465 111.32 -126.25 108.41  1.1159
IC HX   C2   *C3  HY   1.1159 108.41 -114.81 107.61  1.1132
IC C2   C3   O31  C31  1.5508 111.32 -117.52 117.59  1.3317
IC C3   O31  C31  C32  1.4465 117.59 -177.93 109.00  1.5333
IC C32  O31  *C31 O32  1.5333 109.00 -179.19 126.42  1.2107
IC O31  C31  C32  C33  1.3317 109.00 -176.00 111.40  1.5440
IC C33  C31  *C32 H2X  1.5440 111.40  120.79 108.80  1.1093
IC H2X  C31  *C32 H2Y  1.1093 108.80  118.57 108.70  1.1101
IC C21  C22  C23  C24  1.5303 109.53  168.08 112.83  1.5322
IC C24  C22  *C23 H3R  1.5322 112.83 -119.08 109.34  1.1146
IC H3R  C22  *C23 H3S  1.1146 109.34 -118.17 109.92  1.1133
IC C22  C23  C24  C25  1.5428 112.83  179.85 112.06  1.5333
IC C25  C23  *C24 H4R  1.5333 112.06  120.31 108.77  1.1150
IC H4R  C23  *C24 H4S  1.1150 108.77  117.76 110.16  1.1129
IC C23  C24  C25  C26  1.5322 112.06  172.89 112.33  1.5326
IC C26  C24  *C25 H5R  1.5326 112.33 -120.75 109.47  1.1135
IC H5R  C24  *C25 H5S  1.1135 109.47 -117.79 109.27  1.1131
IC C24  C25  C26  C27  1.5333 112.33  175.30 112.46  1.5342
IC C27  C25  *C26 H6R  1.5342 112.46  121.40 108.94  1.1138
IC H6R  C25  *C26 H6S  1.1138 108.94  117.47 109.32  1.1131
IC C25  C26  C27  C28  1.5326 112.46  176.92 112.22  1.5391
IC C28  C26  *C27 H7R  1.5391 112.22 -121.53 108.81  1.1141
IC H7R  C26  *C27 H7S  1.1141 108.81 -117.10 108.50  1.1141
IC C26  C27  C28  C29  1.5342 112.22  177.27 111.34  1.5073
IC C29  C27  *C28 H8R  1.5073 111.34  119.85 107.24  1.1140
IC H8R  C27  *C28 H8S  1.1140 107.24  115.81 109.06  1.1117
IC C27  C28  C29  C210 1.5391 111.34 -141.40 127.31  1.3462
IC C210 C28  *C29 H91  1.3462 127.31 -176.71 114.35  1.1001
IC C28  C29  C210 C211 1.5073 127.31    1.24 127.43  1.5089
IC C211 C29  *C21 H101 1.5089 127.43  179.21 118.33  1.1011
IC C29  C210 C211 C212 1.3462 127.43 -120.91 110.88  1.5393
IC C212 C210 *C21 H11R 1.5393 110.88  121.06 112.51  1.1124
IC H11R C210 *C21 H11S 1.1124 112.51  119.00 109.81  1.1127
IC C210 C211 C212 C213 1.5089 110.88 -176.36 112.76  1.5347
IC C213 C211 *C21 H12R 1.5347 112.76 -120.93 109.33  1.1142
IC H12R C211 *C21 H12S 1.1142 109.33 -118.17 109.94  1.1138
IC C211 C212 C213 C214 1.5393 112.76 -179.47 112.21  1.5338
IC C214 C212 *C21 H13R 1.5338 112.21  121.29 109.31  1.1130
IC H13R C212 *C21 H13S 1.1130 109.31  117.74 109.05  1.1131
IC C212 C213 C214 C215 1.5347 112.21 -178.99 112.92  1.5339
IC C215 C213 *C21 H14R 1.5339 112.92 -121.37 109.00  1.1134
IC H14R C213 *C21 H14S 1.1134 109.00 -117.34 109.08  1.1132
IC C213 C214 C215 C216 1.5338 112.92  179.95 112.20  1.5339
IC C216 C214 *C21 H15R 1.5339 112.20  121.17 109.14  1.1131
IC H15R C214 *C21 H15S 1.1131 109.14  117.63 109.22  1.1132
IC C214 C215 C216 C217 1.5339 112.20  179.53 112.96  1.5328
IC C217 C215 *C21 H16R 1.5328 112.96 -121.41 109.07  1.1135
IC H16R C215 *C21 H16S 1.1135 109.07 -117.43 109.05  1.1130
```

```
IC C215 C216 C217 C218 1.5339  112.96 -179.21  113.03   1.5305
IC C218 C216 *C21 H17R 1.5305  113.03  121.55  108.80   1.1140
IC H17R C216 *C21 H17S 1.1140  108.80  116.88  108.83   1.1142
IC C216 C217 C218 H18R 1.5328  113.03   60.41  110.37   1.1113
IC H18R C217 *C21 H18S 1.1113  110.37 -119.78  110.49   1.1115
IC H18R C217 *C21 H18T 1.1113  110.37  120.07  110.59   1.1111
IC C31  C32  C33  C34  1.5333  111.40  179.66  112.54   1.5345
IC C34  C32  *C33 H3X  1.5345  112.54 -121.73  109.66   1.1133
IC H3X  C32  *C33 H3Y  1.1133  109.66 -117.45  109.37   1.1151
IC C32  C33  C34  C35  1.5440  112.54  178.40  112.54   1.5346
IC C35  C33  *C34 H4X  1.5346  112.54  121.75  110.03   1.1131
IC H4X  C33  *C34 H4Y  1.1131  110.03  117.75  108.84   1.1139
IC C33  C34  C35  C36  1.5345  112.54 -175.14  112.09   1.5349
IC C36  C34  *C35 H5X  1.5349  112.09 -122.26  109.27   1.1127
IC H5X  C34  *C35 H5Y  1.1127  109.27 -117.42  109.08   1.1138
IC C34  C35  C36  C37  1.5346  112.09  174.19  113.84   1.5368
IC C37  C35  *C36 H6X  1.5368  113.84  122.38  109.13   1.1124
IC H6X  C35  *C36 H6Y  1.1124  109.13  117.02  108.50   1.1143
IC C35  C36  C37  C38  1.5349  113.84   65.26  113.87   1.5343
IC C38  C36  *C37 H7X  1.5343  113.87  120.83  108.55   1.1137
IC H7X  C36  *C37 H7Y  1.1137  108.55  116.91  109.10   1.1132
IC C36  C37  C38  C39  1.5368  113.87  178.14  112.45   1.5354
IC C39  C37  *C38 H8X  1.5354  112.45  121.43  109.97   1.1123
IC H8X  C37  *C38 H8Y  1.1123  109.97  117.71  108.91   1.1127
IC C37  C38  C39  C310 1.5343  112.45 -176.66  111.96   1.5320
IC C310 C38  *C39 H9X  1.5320  111.96  120.68  109.20   1.1133
IC H9X  C38  *C39 H9Y  1.1133  109.20  117.81  109.34   1.1127
IC C38  C39  C310 C311 1.5354  111.96  178.35  113.81   1.5336
IC C311 C39  *C31 H10X 1.5336  113.81 -120.14  108.22   1.1126
IC H10X C39  *C31 H10Y 1.1126  108.22 -117.07  109.45   1.1132
IC C39  C310 C311 C312 1.5320  113.81 -175.46  111.16   1.5334
IC C312 C310 *C31 H11X 1.5334  111.16  120.27  109.12   1.1138
IC H11X C310 *C31 H11Y 1.1138  109.12  118.20  110.02   1.1119
IC C310 C311 C312 C313 1.5336  111.16  173.60  113.47   1.5330
IC C313 C311 *C31 H12X 1.5330  113.47 -120.74  108.01   1.1140
IC H12X C311 *C31 H12Y 1.1140  108.01 -116.85  109.45   1.1130
IC C311 C312 C313 C314 1.5334  113.47 -174.75  111.86   1.5335
IC C314 C312 *C31 H13X 1.5335  111.86  120.28  108.66   1.1135
IC H13X C312 *C31 H13Y 1.1135  108.66  118.03  110.08   1.1125
IC C312 C313 C314 C315 1.5330  111.86  175.21  113.05   1.5325
IC C315 C313 *C31 H14X 1.5325  113.05 -120.81  108.37   1.1133
IC H14X C313 *C31 H14Y 1.1133  108.37 -117.18  109.40   1.1131
IC C313 C314 C315 C316 1.5335  113.05 -177.76  112.89   1.5300
IC C316 C314 *C31 H15X 1.5300  112.89  121.41  108.55   1.1149
IC H15X C314 *C31 H15Y 1.1149  108.55  117.05  109.21   1.1136
IC C314 C315 C316 H16X 1.5325  112.89   57.15  110.07   1.1113
IC H16X C315 *C31 H16Y 1.1113  110.07 -119.27  110.55   1.1106
IC H16X C315 *C31 H16Z 1.1113  110.07  120.81  110.70   1.1116

!The following two residues (PALM and PCGL) and the two subsequent
!patches (EST1 and EST2) are a modular way to create DPPC.
!See the comments with EST1 and EST2 for more details. adm jr., Jul 99

RESI PALM        -1.00 ! Palmitate
                       ! based on methylsulfate

GROUP                                  O1  O2 (-)
ATOM C1   CL      0.62 !                \\ /
ATOM O1   OCL    -0.76 !                 C1
ATOM O2   OCL    -0.76 !                  |
```

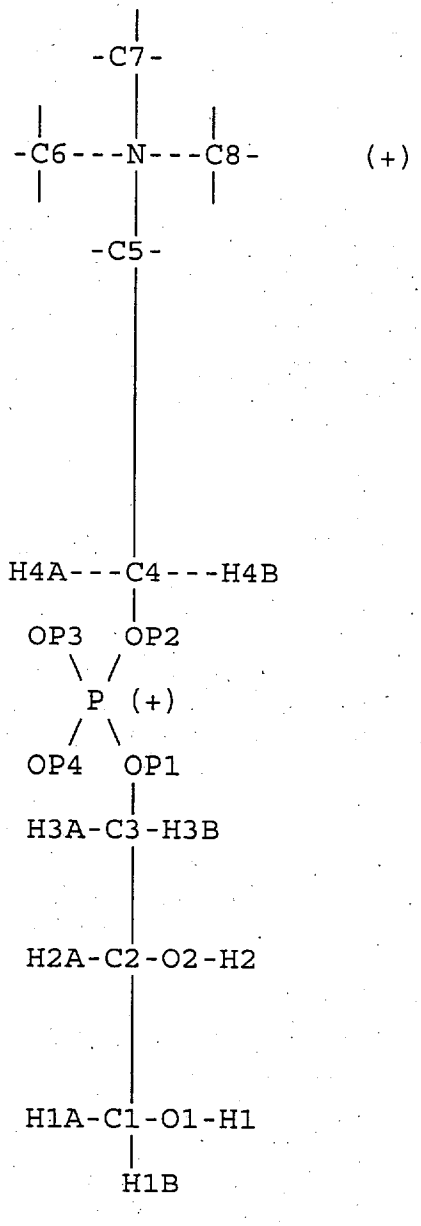
```
                                !
ATOM C2    CTL2    -0.28 !          H2A-C2-H2B
ATOM H2A   HAL2     0.09 !
ATOM H2B   HAL2     0.09 !
GROUP                    !
ATOM C3    CTL2    -0.18 !          H3A-C3-H3B
ATOM H3A   HAL2     0.09 !
ATOM H3B   HAL2     0.09 !
GROUP                    !
ATOM C4    CTL2    -0.18 !          H4A-C4-H4B
ATOM H4A   HAL2     0.09 !
ATOM H4B   HAL2     0.09 !
GROUP                    !
ATOM C5    CTL2    -0.18 !          H5A-C5-H5B
ATOM H5A   HAL2     0.09 !
ATOM H5B   HAL2     0.09 !
GROUP                    !
ATOM C6    CTL2    -0.18 !          H6A-C6-H6B
ATOM H6A   HAL2     0.09 !
ATOM H6B   HAL2     0.09 !
GROUP                    !
ATOM C7    CTL2    -0.18 !          H7A-C7-H7B
ATOM H7A   HAL2     0.09 !
ATOM H7B   HAL2     0.09 !
GROUP                    !
ATOM C8    CTL2    -0.18 !          H8A-C8-H8B
ATOM H8A   HAL2     0.09 !
ATOM H8B   HAL2     0.09 !
GROUP                    !
ATOM C9    CTL2    -0.18 !          H9A-C9-H9B
ATOM H9A   HAL2     0.09 !
ATOM H9B   HAL2     0.09 !
GROUP                    !
ATOM C10   CTL2    -0.18 !         H10A-C10-H10B
ATOM H10A  HAL2     0.09 !
ATOM H10B  HAL2     0.09 !
GROUP                    !
ATOM C11   CTL2    -0.18 !         H11A-C11-H11B
ATOM H11A  HAL2     0.09 !
ATOM H11B  HAL2     0.09 !
GROUP                    !
ATOM C12   CTL2    -0.18 !         H12A-C12-H12B
ATOM H12A  HAL2     0.09 !
ATOM H12B  HAL2     0.09 !
GROUP                    !
ATOM C13   CTL2    -0.18 !         H13A-C13-H13B
ATOM H13A  HAL2     0.09 !
ATOM H13B  HAL2     0.09 !
GROUP                    !
ATOM C14   CTL2    -0.18 !         H14A-C14-H14B
ATOM H14A  HAL2     0.09 !
ATOM H14B  HAL2     0.09 !
GROUP                    !
ATOM C15   CTL2    -0.18 !         H15A-C15-H15B
ATOM H15A  HAL2     0.09 !
ATOM H15B  HAL2     0.09 !
GROUP                    !
ATOM C16   CTL3    -0.27 !         H16A-C16-H16B
ATOM H16A  HAL3     0.09 !
ATOM H16B  HAL3     0.09 !             H16C
```

```
ATOM H16C HAL3    0.09 !

BOND  C1  O1  C1  O2
BOND  C1  C2  C2  H2A  C2  H2B
BOND  C2  C3  C3  H3A  C3  H3B
BOND  C3  C4  C4  H4A  C4  H4B
BOND  C4  C5  C5  H5A  C5  H5B
BOND  C5  C6  C6  H6A  C6  H6B
BOND  C6  C7  C7  H7A  C7  H7B
BOND  C7  C8  C8  H8A  C8  H8B
BOND  C8  C9  C9  H9A  C9  H9B
BOND  C9  C10 C10 H10A C10 H10B
BOND  C10 C11 C11 H11A C11 H11B
BOND  C11 C12 C12 H12A C12 H12B
BOND  C12 C13 C13 H13A C13 H13B
BOND  C13 C14 C14 H14A C14 H14B
BOND  C14 C15 C15 H15A C15 H15B
BOND  C15 C16 C16 H16A C16 H16B C16 H16C
IMPR C1 O1 C2 O2
ACCE  O1
ACCE  O2
!IC table insufficent to create cartesian coordinates
IC O1   C2   *C1  O2   0.0000   0.00  180.00   0.00   0.0000
IC O1   C1   C2   C3   0.0000   0.00  180.00   0.00   0.0000
IC C3   C1   *C2  H2A  0.0000   0.00  120.00   0.00   0.0000
IC H2A  C1   *C2  H2B  0.0000   0.00 -120.00   0.00   0.0000
IC C1   C2   C3   C4   0.0000   0.00  180.00   0.00   0.0000
IC C4   C2   *C3  H3A  0.0000   0.00  120.00   0.00   0.0000
IC H3A  C2   *C3  H3B  0.0000   0.00 -120.00   0.00   0.0000
IC C2   C3   C4   C5   0.0000   0.00  180.00   0.00   0.0000
IC C5   C3   *C4  H4A  0.0000   0.00  120.00   0.00   0.0000
IC H4A  C3   *C4  H4B  0.0000   0.00 -120.00   0.00   0.0000
IC C3   C4   C5   C6   0.0000   0.00  180.00   0.00   0.0000
IC C6   C4   *C5  H5A  0.0000   0.00  120.00   0.00   0.0000
IC H5A  C4   *C5  H5B  0.0000   0.00 -120.00   0.00   0.0000
IC C4   C5   C6   C7   0.0000   0.00  180.00   0.00   0.0000
IC C7   C5   *C6  H6A  0.0000   0.00  120.00   0.00   0.0000
IC H6A  C5   *C6  H6B  0.0000   0.00 -120.00   0.00   0.0000
IC C5   C6   C7   C8   0.0000   0.00  180.00   0.00   0.0000
IC C8   C6   *C7  H7A  0.0000   0.00  120.00   0.00   0.0000
IC H7A  C6   *C7  H7B  0.0000   0.00 -120.00   0.00   0.0000
IC C6   C7   C8   C9   0.0000   0.00  180.00   0.00   0.0000
IC C9   C7   *C8  H8A  0.0000   0.00  120.00   0.00   0.0000
IC H8A  C7   *C8  H8B  0.0000   0.00 -120.00   0.00   0.0000
IC C7   C8   C9   C10  0.0000   0.00  180.00   0.00   0.0000
IC C10  C8   *C9  H9A  0.0000   0.00  120.00   0.00   0.0000
IC H9A  C8   *C9  H9B  0.0000   0.00 -120.00   0.00   0.0000
IC C8   C9   C10  C11  0.0000   0.00  180.00   0.00   0.0000
IC C11  C9   *C10 H10A 0.0000   0.00  120.00   0.00   0.0000
IC H10A C9   *C10 H10B 0.0000   0.00 -120.00   0.00   0.0000
IC C9   C10  C11  C12  0.0000   0.00  180.00   0.00   0.0000
IC C12  C10  *C11 H11A 0.0000   0.00  120.00   0.00   0.0000
IC H11A C10  *C11 H11B 0.0000   0.00 -120.00   0.00   0.0000
IC C10  C11  C12  C13  0.0000   0.00  180.00   0.00   0.0000
IC C13  C11  *C12 H12A 0.0000   0.00  120.00   0.00   0.0000
IC H12A C11  *C12 H12B 0.0000   0.00 -120.00   0.00   0.0000
IC C11  C12  C13  C14  0.0000   0.00  180.00   0.00   0.0000
IC C14  C12  *C13 H13A 0.0000   0.00  120.00   0.00   0.0000
IC H13A C12  *C13 H13B 0.0000   0.00 -120.00   0.00   0.0000
IC C12  C13  C14  C15  0.0000   0.00  180.00   0.00   0.0000
```

```
IC C15   C13   *C14 H14A 0.0000    0.00  120.00    0.00   0.0000
IC H14A C13   *C14 H14B 0.0000    0.00 -120.00    0.00   0.0000
IC C13   C14   C15   C16  0.0000    0.00  180.00    0.00   0.0000
IC C16   C14   *C15 H15A 0.0000    0.00  120.00    0.00   0.0000
IC H15A C14   *C15 H15B 0.0000    0.00 -120.00    0.00   0.0000
IC C14   C15   C16   H16A 0.0000    0.00  180.00    0.00   0.0000
IC H16A C15   *C16 H16B 0.0000    0.00  120.00    0.00   0.0000
IC H16A C15   *C16 H16C 0.0000    0.00 -120.00    0.00   0.0000

RESI PCGL          0.00 ! glycerolphosphorylcholine
                        ! nomenclature for creation of DPPC
GROUP                   ! from PALM and PCGL via patches EST1 and EST2
ATOM N     NTL    -0.60 !
ATOM C5    CTL2   -0.10 !
ATOM C6    CTL5   -0.35 !
ATOM C7    CTL5   -0.35 !
ATOM C8    CTL5   -0.35 !
ATOM H5A   HL      0.25 !
ATOM H5B   HL      0.25 !
ATOM H6A   HL      0.25 !
ATOM H6B   HL      0.25 !
ATOM H6C   HL      0.25 !
ATOM H7A   HL      0.25 !
ATOM H7B   HL      0.25 !
ATOM H7C   HL      0.25 !
ATOM H8A   HL      0.25 !
ATOM H8B   HL      0.25 !
ATOM H8C   HL      0.25 !
GROUP                   !
ATOM C4    CTL2   -0.08 !
ATOM H4A   HAL2    0.09 !
ATOM H4B   HAL2    0.09 !
ATOM P     PL      1.50 !
ATOM OP3   O2L    -0.78 !
ATOM OP4   O2L    -0.78 !
ATOM OP1   OSL    -0.57 !
ATOM OP2   OSL    -0.57 !
ATOM C3    CTL2   -0.08 !
ATOM H3A   HAL2    0.09 !
ATOM H3B   HAL2    0.09 !
GROUP                   !
ATOM C2    CTL1    0.14 !
ATOM H2A   HAL1    0.09 !
ATOM O2    OHL    -0.66 !
ATOM H2    HOL     0.43 !
GROUP                   !
ATOM C1    CTL2    0.05 !
ATOM H1A   HAL2    0.09 !
ATOM H1B   HAL2    0.09 !
ATOM O1    OHL    -0.66 !
ATOM H1    HOL     0.43 !
BOND N    C5    N    C6     N    C7     N    C8
BOND C5   C4    C4   OP2    OP2  P      P    OP1
BOND P    OP3   P    OP4
BOND OP1  C3    C3   C2     C2   C1
BOND C2   O2    C1   O1
BOND O1   H1    O2   H2
BOND C1   H1A   C1   H1B
BOND C2   H2A
BOND C3   H3A   C3   H3B
```



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BOND C4   H4A   C4   H4B
BOND C5   H5A   C5   H5B
BOND C6   H6A   C6   H6B   C6   H6C
BOND C7   H7A   C7   H7B   C7   H7C
BOND C8   H8A   C8   H8B   C8   H8C
!IC table insufficent to create cartesian coordinates
IC C6    C5    *N    C7    0.0000    0.00  120.00    0.00    0.0000
IC C6    C5    *N    C8    0.0000    0.00 -120.00    0.00    0.0000
IC C6    N     C5    C4    0.0000    0.00  180.00    0.00    0.0000
IC C4    N     *C5   H5A   0.0000    0.00  120.00    0.00    0.0000
IC C4    N     *C5   H5B   0.0000    0.00 -120.00    0.00    0.0000
IC C5    N     C6    H6A   0.0000    0.00  180.00    0.00    0.0000
IC H6A   N     *C6   H6B   0.0000    0.00  120.00    0.00    0.0000
IC H6A   N     *C6   H6C   0.0000    0.00 -120.00    0.00    0.0000
IC C5    N     C7    H7A   0.0000    0.00  180.00    0.00    0.0000
IC H7A   N     *C7   H7B   0.0000    0.00  120.00    0.00    0.0000
IC H7A   N     *C7   H7C   0.0000    0.00 -120.00    0.00    0.0000
IC C5    N     C8    H8A   0.0000    0.00  180.00    0.00    0.0000
IC H8A   N     *C8   H8B   0.0000    0.00  120.00    0.00    0.0000
IC H8A   N     *C8   H8C   0.0000    0.00 -120.00    0.00    0.0000
IC N     C5    C4    OP2   0.0000    0.00  180.00    0.00    0.0000
IC OP2   C5    *C4   H4A   0.0000    0.00  120.00    0.00    0.0000
IC OP2   C5    *C4   H4B   0.0000    0.00 -120.00    0.00    0.0000
IC C5    C4    OP2   P     0.0000    0.00  180.00    0.00    0.0000
IC C4    OP2   P     OP1   0.0000    0.00  180.00    0.00    0.0000
IC OP1   OP2   *P    OP3   0.0000    0.00  120.00    0.00    0.0000
IC OP1   OP2   *P    OP4   0.0000    0.00 -120.00    0.00    0.0000
IC OP2   P     OP1   C3    0.0000    0.00  180.00    0.00    0.0000
IC P     OP1   C3    C2    0.0000    0.00  180.00    0.00    0.0000
IC C2    OP1   *C3   H3A   0.0000    0.00  120.00    0.00    0.0000
IC C2    OP1   *C3   H3B   0.0000    0.00 -120.00    0.00    0.0000
IC OP1   C3    C2    C1    0.0000    0.00  180.00    0.00    0.0000
IC C1    C3    *C2   O2    0.0000    0.00  120.00    0.00    0.0000
IC C1    C3    *C2   H2A   0.0000    0.00 -120.00    0.00    0.0000
IC C3    C2    O2    H2    0.0000    0.00  180.00    0.00    0.0000
IC C3    C2    C1    O1    0.0000    0.00  180.00    0.00    0.0000
IC O1    C2    *C1   H1A   0.0000    0.00  120.00    0.00    0.0000
IC O1    C2    *C1   H1B   0.0000    0.00 -120.00    0.00    0.0000
IC C2    C1    O1    H1    0.0000    0.00  180.00    0.00    0.0000

PRES EST1         0.00 !patch to link O1 of PCGL to C1 of PALM
! residue 1 is PCGL, residue 2 is PALM
DELETE ATOM 1H1
DELETE ATOM 2O2
ATOM 1C1  CTL2  -0.05 !      1H1A--1C1--1H1B
ATOM 1H1A HAL2   0.09 !                |
ATOM 1H1B HAL2   0.09 !                |
ATOM 1O1  OSL   -0.34 !        2O1   1O1
ATOM 2C1  CL     0.63 !          \\  /
ATOM 2O1  OBL   -0.52 !           2C1
ATOM 2C2  CTL2  -0.08 !            |
ATOM 2H2A HAL2   0.09 !   2H2A--2C2--2H2B
ATOM 2H2B HAL2   0.09 !            |
BOND 1O1  2C1

PRES EST2         0.00 !patch to link O2 of PCGL to C1 of PALM
! residue 1 is PCGL, residue 2 is PALM
DELETE ATOM 1H2
DELETE ATOM 2O2
GROUP
```

```
ATOM 1C2   CTL1    0.04 !      1H2A--1C2--
ATOM 1H2A  HAL1    0.09 !              |
ATOM 1O2   OSL    -0.34 !        2O1  1O2
ATOM 2C1   CL      0.63 !         \\ /
ATOM 2O1   OBL    -0.52 !          2C1
ATOM 2C2   CTL2   -0.08 !           |
ATOM 2H2A  HAL2    0.09 !  2H2A--2C2--2H2B
ATOM 2H2B  HAL2    0.09 !           |
BOND 1O2   2C1
```

```
END
```

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*  \\\\\\\ CHARMM27 All-Hydrogen Lipid Parameter File ///////
*

!Feller, S.E. and MacKerell, Jr., A.D. An Improved Empirical Potential
!Energy Function for Molecular Simulations of Phospholipids
!
!additional references
!
!Schlenkrich, M., Brickmann, J., MacKerell, Jr., A.D., and Karplus, M.
!Empirical Potential Energy Function for Phospholipids: Criteria for
!Parameter Optimization and Applications, in "Biological Membranes: A
!Molecular Perspective from Computation and Experiment," K.M. Merz and
!B. Roux, Eds. Birkhauser, Boston, 1996, pp 31-81.
!
!ALKANES
!
!Yin, D. and MacKerell, Jr. A.D. Combined Ab initio/Empirical Approach
!for the Optimization of Lennard-Jones Parameters. Journal of
!Computational Chemistry, 1998, 19: 334-338.
!
!ALKENES
!
!Feller, S.E., Yin, D., Pastor, R.W., and MacKerell, Jr., A.D.,
!Molecular Dynamics Simulation of Unsaturated Lipids at Low Hydration:
!Parameterization and Comparison with Diffraction Studies.  Biophysical
!Journal, 73:2269-2279, 1997.
!
!new PHOSPHATE
!
!MacKerell, Jr., A.D. Influence of Water and Sodium on the Energetics
!of Dimethylphosphate and its Implications For DNA Structure, Journal
!de Chimie Physique, 1997, 94: 1436-1447.
!
!IONS
!
!all ions from Roux and coworkers
!
!Sodium
!
!Beglov, D. and Roux, B., Finite Representation of an Infinite
!Bulk System: Solvent Boundary Potential for Computer Simulations,
!Journal of Chemical Physics, 1994, 100: 9050-9063
!

BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
!
CTL3   CL    200.0       1.522    ! methyl acetate
CTL2   CL    200.0       1.522    ! methyl acetate
CTL1   CL    200.0       1.522    ! methyl acetate
OBL    CL    750.0       1.220    ! methyl acetate
OCL    CL    525.0       1.260    ! acetate, protein
OSL    CL    150.0       1.334    ! methyl acetate
OHL    CL    230.0       1.40     ! methyl acetate
```

```
HOL    OHL    545.0       0.960   ! acetic acid
CTL1   HAL1   309.00      1.111   ! alkanes, 3/92
CTL2   HAL2   309.00      1.111   ! alkanes, 4/98
CTL3   HAL3   322.00      1.111   ! alkanes, 4/98
CTL3   OSL    340.0       1.43    ! phosphate
CTL2   OSL    340.0       1.43    ! phosphate
CTL1   OSL    340.0       1.43    ! phosphate
OSL    PL     270.0       1.60    ! phosphate
O2L    PL     580.0       1.48    ! phosphate
OHL    PL     237.0       1.59    ! phosphate
NH3L   HCL    410.0       1.04    ! ethanolamine
NH3L   CTL2   261.0       1.51    ! ethanolamine
NTL    CTL2   215.00      1.51    ! tetramethylammonium
NTL    CTL5   215.00      1.51    ! tetramethylammonium
CTL5   HL     300.00      1.08    ! tetramethylammonium
CTL2   HL     300.00      1.08    ! tetramethylammonium
CTL1   CTL1   222.500     1.500   ! alkanes, 3/92
CTL1   CTL2   222.500     1.538   ! alkanes, 3/92
CTL1   CTL3   222.500     1.538   ! alkanes, 3/92
CTL2   CTL2   222.500     1.530   ! alkanes, 3/92
CTL2   CTL3   222.500     1.528   ! alkanes, 3/92
CTL3   CTL3   222.500     1.530   ! alkanes, 3/92
OHL    CTL1   428.0       1.420   !  glycerol
OHL    CTL2   428.0       1.420   !  glycerol
OHL    CTL3   428.0       1.420   !  glycerol
SL     O2L    540.0       1.448   ! methylsulfate
SL     OSL    250.0       1.575   ! methylsulfate
HT     HT       0.0       1.5139  ! from TIPS3P geometry (for SHAKE w/PARAM)
HT     OT     450.0       0.9572  ! from TIPS3P geometry
CEL2   CEL2   510.000     1.330   ! ethene yin,adm jr., 12/95
HEL2   CEL2   365.000     1.100   ! propene; from ethene, yin,adm jr., 12/95
CEL1   CTL3   383.000     1.504   ! butene, yin,adm jr., 12/95
CEL1   CEL2   500.000     1.342   ! propene, yin,adm jr., 12/95
HEL1   CEL1   360.500     1.100   ! propene, yin,adm jr., 12/95
CEL1   CTL2   365.000     1.502   ! butene; from propene, yin,adm jr., 12/95
CEL1   CEL1   440.000     1.340   ! butene, yin,adm jr., 12/95

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
!
OBL   CL    CTL3     70.0      125.0     20.0    2.442  ! methyl acetate
OBL   CL    CTL2     70.0      125.0     20.0    2.442  ! methyl acetate
OBL   CL    CTL1     70.0      125.0     20.0    2.442  ! methyl acetate
OSL   CL    OBL      90.0      125.9    160.0    2.2576 ! acetic acid
CL    OSL   CTL1     40.0      109.6     30.0    2.2651 ! methyl acetate
CL    OSL   CTL2     40.0      109.6     30.0    2.2651 ! methyl acetate
CL    OSL   CTL3     40.0      109.6     30.0    2.2651 ! methyl acetate
HAL2  CTL2  CL       33.00     109.50   30.00    2.163  ! methyl acetate
HAL3  CTL3  CL       33.00     109.50   30.00    2.163  ! methyl acetate
CTL2  CTL2  CL       52.0      108.00   ! alkane
```

```
CTL3  CTL2  CL      52.0     108.00   ! alkane
OSL   CL    CTL3    55.0     109.0    20.00   2.3260 ! methyl acetate
OSL   CL    CTL2    55.0     109.0    20.00   2.3260 ! methyl acetate
OHL   CL    OBL     50.0     123.0    210.0   2.2620 ! acetic acid
OCL   CL    CTL2    40.0     118.0     50.0   2.3880 ! acetate
OCL   CL    CTL3    40.0     118.0     50.0   2.3880 ! acetate
OCL   CL    OCL    100.0     124.0     70.0   2.2250 ! acetate
OHL   CL    CTL3    55.0     110.50   ! acetic acid
OHL   CL    CTL2    55.0     110.50   ! acetic acid
HOL   OHL   CL      55.0     115.0    ! acetic acid
OSL   CTL1  CTL2    75.700   110.10   ! acetic acid
OSL   CTL1  CTL3    75.700   110.10   ! acetic acid
OSL   CTL2  CTL1    75.700   110.10   ! acetic acid
OSL   CTL2  CTL2    75.700   110.10   ! acetic acid
OSL   CTL2  CTL3    75.700   110.10   ! acetic acid
HAL2  CTL2  HAL2    35.500   109.00    5.40   1.80200 ! alkane, 3/92
HAL3  CTL3  HAL3    35.500   108.40    5.40   1.80200 ! alkane, 3/92
HAL1  CTL1  OSL     60.0     109.5    ! phosphate
HAL2  CTL2  OSL     60.0     109.5    ! phosphate
HAL3  CTL3  OSL     60.0     109.5    ! phosphate
CTL2  OSL   PL      20.0     120.0    35.0    2.33   ! phosphate
CTL3  OSL   PL      20.0     120.0    35.0    2.33   ! phosphate
HOL   OHL   PL      30.0     115.0    40.0    2.30   ! phosphate
OSL   PL    OSL     80.0     104.3    ! phosphate
OSL   PL    O2L     98.9     111.6    ! phosphate
OSL   PL    OHL     48.1     108.0    ! phosphate
O2L   PL    O2L    120.0     120.0    ! phosphate
O2L   PL    OHL     98.9     108.23   ! phosphate
NTL   CTL2  HL      40.0     109.5    27.     2.13   ! tetramethylammonium
NTL   CTL5  HL      40.0     109.5    27.     2.13   ! tetramethylammonium
HL    CTL2  HL      24.0     109.50   28.     1.767  ! tetramethylammonium
HL    CTL5  HL      24.0     109.50   28.     1.767  ! tetramethylammonium
CTL5  NTL   CTL2    60.0     109.5    26.     2.466  ! tetramethylammonium
CTL5  NTL   CTL5    60.0     109.5    26.     2.466  ! tetramethylammonium
HL    CTL2  CTL2    33.430   110.10   22.53   2.179  ! alkane
HL    CTL2  CTL3    33.430   110.10   22.53   2.179  ! alkane
HAL1  CTL1  CTL1    34.500   110.10   22.53   2.179  ! alkane, 3/92
HAL1  CTL1  CTL2    34.500   110.10   22.53   2.179  ! alkane, 3/92
HAL1  CTL1  CTL3    34.500   110.10   22.53   2.179  ! alkane, 3/92
HAL2  CTL2  CTL1    26.500   110.10   22.53   2.179  ! alkane, 4/98
HAL2  CTL2  CTL2    26.500   110.10   22.53   2.179  ! alkane, 4/98
HAL2  CTL2  CTL3    34.600   110.10   22.53   2.179  ! alkane, 4/98
HAL3  CTL3  CTL1    33.430   110.10   22.53   2.179  ! alkane, 4/98
HAL3  CTL3  CTL2    34.600   110.10   22.53   2.179  ! alkane, 4/98
HAL3  CTL3  CTL3    37.500   110.10   22.53   2.179  ! alkane, 4/98
NTL   CTL2  CTL2    67.7     115.00   ! tetramethylammonium
NTL   CTL2  CTL3    67.7     115.00   ! tetramethylammonium
HCL   NH3L  CTL2    33.0     109.50    4.00   2.056  ! ethanolamine
HCL   NH3L  HCL     41.0     109.50   ! ethanolamine
NH3L  CTL2  CTL2    67.7     110.00   ! ethanolamine
NH3L  CTL2  HAL2    45.0     107.50   35.00   2.0836 ! ethanolamine
CTL1  CTL1  CTL1    53.350   111.00    8.00   2.561  ! alkane, 3/92
CTL1  CTL1  CTL2    58.350   113.50   11.16   2.561  ! glycerol
CTL1  CTL1  CTL3    53.350   108.50    8.00   2.561  ! alkane, 3/92
CTL1  CTL2  CTL1    58.350   113.50   11.16   2.561  ! glycerol
CTL1  CTL2  CTL2    58.350   113.50   11.16   2.561  ! glycerol
CTL1  CTL2  CTL3    58.350   113.50   11.16   2.561  ! glycerol
CTL2  CTL1  CTL2    58.350   113.50   11.16   2.561  ! glycerol
CTL2  CTL1  CTL3    58.350   113.50   11.16   2.561  ! glycerol
CTL2  CTL2  CTL2    58.350   113.60   11.16   2.561  ! alkane, 3/92
```

```
CTL2  CTL2  CTL3    58.000     115.00     8.00   2.561  ! alkane, 3/92
HOL   OHL   CTL1    57.500     106.00   ! glycerol
HOL   OHL   CTL2    57.500     106.00   ! glycerol
HOL   OHL   CTL3    57.500     106.00   ! glycerol
OHL   CTL1  CTL2    75.700     110.10   ! glycerol
OHL   CTL2  CTL1    75.700     110.10   ! glycerol
OHL   CTL2  CTL2    75.700     110.10   ! glycerol
OHL   CTL2  CTL3    75.700     110.10   ! glycerol
OHL   CTL1  HAL1    45.900     108.89   ! glycerol
OHL   CTL2  HAL2    45.900     108.89   ! glycerol
OHL   CTL3  HAL3    45.900     108.89   ! glycerol
O2L   SL    O2L    130.0       109.47  35.0    2.45 ! methylsulfate
O2L   SL    OSL     85.0        98.0                ! methylsulfate
CTL2  OSL   SL      15.0       109.0   27.00   1.90 ! methylsulfate
CTL3  OSL   SL      15.0       109.0   27.00   1.90 ! methylsulfate
HT    OT    HT      55.0       104.52   ! FROM TIPS3P GEOMETRY
CEL1  CEL1  CTL2    48.00      123.50   ! from 2-butene, yin,adm jr., 12/95
CEL1  CEL1  CTL3    48.00      123.50   ! 2-butene, yin,adm jr., 12/95
CEL2  CEL1  CTL2    48.00      126.00   ! 1-butene; from propene, yin,adm jr., 12/95
CEL2  CEL1  CTL3    47.00      125.20   ! propene, yin,adm jr., 12/95
HEL1  CEL1  CEL1    52.00      119.50   ! 2-butene, yin,adm jr., 12/95
HEL1  CEL1  CEL2    42.00      118.00   ! propene, yin,adm jr., 12/95
HEL1  CEL1  CTL2    40.00      116.00   ! 1-butene; from propene, yin,adm jr., 12/95
HEL1  CEL1  CTL3    22.00      117.00   ! propene, yin,adm jr., 12/95
HEL2  CEL2  CEL1    45.00      120.50   ! propene, yin,adm jr., 12/95
HEL2  CEL2  CEL2    55.50      120.50   ! ethene, yin,adm jr., 12/95
HEL2  CEL2  HEL2    19.00      119.00   ! propene, yin,adm jr., 12/95
CEL1  CTL2  CTL2    32.00      112.20   ! 1-butene; from propene, yin,adm jr., 12/95
CEL1  CTL2  CTL3    32.00      112.20   ! 1-butene; from propene, yin,adm jr., 12/95
HAL2  CTL2  CEL1    45.00      111.50   ! 1-butene; from propene, yin,adm jr., 12/95
HAL3  CTL3  CEL1    42.00      111.50   ! 2-butene, yin,adm jr., 12/95

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types                 Kchi    n   delta
!
X     CTL1  OHL   X          0.14    3     0.00 ! glycerol
X     CTL2  OHL   X          0.14    3     0.00 ! glycerol
X     CTL3  OHL   X          0.14    3     0.00 ! glycerol
OBL   CL    CTL2  HAL2       0.00    6   180.00 ! acetic acid
OBL   CL    CTL3  HAL3       0.00    6   180.00 ! acetic acid
OSL   CL    CTL2  HAL2       0.00    6   180.00 ! acetic acid
OSL   CL    CTL3  HAL3       0.00    6   180.00 ! acetic acid
OBL   CL    OSL   CTL1       0.965   1   180.00 ! methyl acetate
OBL   CL    OSL   CTL1       3.85    2   180.00 ! methyl acetate
OBL   CL    OSL   CTL2       0.965   1   180.00 ! methyl acetate
OBL   CL    OSL   CTL2       3.85    2   180.00 ! methyl acetate
OBL   CL    OSL   CTL3       0.965   1   180.00 ! methyl acetate
OBL   CL    OSL   CTL3       3.85    2   180.00 ! methyl acetate
X     CL    OSL   X          2.05    2   180.00 ! methyl acetate
X     CTL2  CL    X          0.05    6   180.00 ! methyl acetate
X     CTL3  CL    X          0.05    6   180.00 ! methyl acetate
X     CL    OHL   X          2.05    2   180.00 ! acetic acid
HAL2  CTL2  CL    OHL        0.00    6   180.00
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HAL3 CTL3 CL   OHL      0.00     6   180.00
OSL  PL   OSL  CTL2     1.20     1   180.00 ! phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL2     0.10     2   180.00 ! phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL2     0.10     3   180.00 ! phosphate, new NA, 4/98, adm jr.
O2L  PL   OSL  CTL2     0.10     3     0.00 ! phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL3     1.20     1   180.00 ! phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL3     0.10     2   180.00 ! phosphate, new NA, 4/98, adm jr.
OSL  PL   OSL  CTL3     0.10     3   180.00 ! phosphate, new NA, 4/98, adm jr.
O2L  PL   OSL  CTL3     0.10     3     0.00 ! phosphate, new NA, 4/98, adm jr.
OHL  PL   OSL  CTL2     0.95     2     0.00 ! terminal phosphate
OHL  PL   OSL  CTL2     0.50     3     0.00 ! terminal phosphate
OHL  PL   OSL  CTL3     0.95     2     0.00 ! terminal phosphate
OHL  PL   OSL  CTL3     0.50     3     0.00 ! terminal phosphate
X    OHL  PL   X        0.30     3     0.00 ! phosphate, new NA, 4/98, adm jr.
X    CTL1 OSL  X        0.00     3     0.00 ! phosphate, new NA, 4/98, adm jr.
X    CTL2 OSL  X        0.00     3     0.00 ! phosphate, new NA, 4/98, adm jr.
X    CTL3 OSL  X        0.00     3     0.00 ! phosphate, new NA, 4/98, adm jr.
CTL3 CTL2 OSL  CL       0.7      1   180.00 ! ethyl acetate, 12/92
CTL2 CTL2 OSL  CL       0.7      1   180.00 ! ethyl acetate, 12/92
CTL3 CTL1 OSL  CL       0.7      1   180.00 ! ethyl acetate, 12/92
CTL2 CTL1 OSL  CL       0.7      1   180.00 ! ethyl acetate, 12/92
CTL1 CTL2 CL   OSL     -0.15     1   180.00 ! methyl propionate, 12/92
CTL1 CTL2 CL   OSL      0.53     2   180.00 ! methyl propionate, 12/92
CTL2 CTL2 CL   OSL     -0.15     1   180.00 ! methyl propionate, 12/92
CTL2 CTL2 CL   OSL      0.53     2   180.00 ! methyl propionate, 12/92
CTL3 CTL2 CL   OSL     -0.15     1   180.00 ! methyl propionate, 12/92
CTL3 CTL2 CL   OSL      0.53     2   180.00 ! methyl propionate, 12/92
X    CTL2 NTL  X        0.26     3     0.00 ! tetramethylammonium
X    CTL5 NTL  X        0.23     3     0.00 ! tetramethylammonium
X    CTL2 NH3L X        0.10     3     0.00 ! ethanolamine
NH3L CTL2 CTL2 OHL      0.7      1   180.00 ! ethanolamine
NH3L CTL2 CTL2 OSL      0.7      1   180.00 ! choline, 12/92
NTL  CTL2 CTL2 OHL      4.3      1   180.00 ! choline, 12/92
NTL  CTL2 CTL2 OHL     -0.4      3   180.00 ! choline, 12/92
NTL  CTL2 CTL2 OSL      3.3      1   180.00 ! choline, 12/92
NTL  CTL2 CTL2 OSL     -0.4      3   180.00 ! choline, 12/92
X    CTL1 CTL1 X        0.200    3     0.00 ! alkane, 3/92
X    CTL1 CTL2 X        0.200    3     0.00 ! alkane, 3/92
X    CTL1 CTL3 X        0.200    3     0.00 ! alkane, 3/92
X    CTL2 CTL2 X        0.1900   3     0.00 ! alkane, 4/98, yin and mackerell
X    CTL2 CTL3 X        0.1600   3     0.00 ! alkane, 4/98, yin and mackerell
X    CTL3 CTL3 X        0.1525   3     0.00 ! alkane, 4/98, adm jr., lower butane
CTL3 CTL2 CTL2 CTL3     0.10     2   180.00 ! alkane, 4/98, adm jr.
CTL3 CTL2 CTL2 CTL3     0.15     4     0.00 ! alkane, 4/98, adm jr.
CTL3 CTL2 CTL2 CTL3     0.10     6   180.00 ! alkane, 4/98, adm jr.
CTL2 CTL2 CTL2 CTL3     0.10     2   180.00 ! alkane, 4/98, adm jr.
CTL2 CTL2 CTL2 CTL3     0.15     4     0.00 ! alkane, 4/98, adm jr.
CTL2 CTL2 CTL2 CTL3     0.10     6   180.00 ! alkane, 4/98, adm jr.
CTL2 CTL2 CTL2 CTL2     0.10     2   180.00 ! alkane, 4/98, adm jr.
CTL2 CTL2 CTL2 CTL2     0.15     4     0.00 ! alkane, 4/98, adm jr.
CTL2 CTL2 CTL2 CTL2     0.10     6   180.00 ! alkane, 4/98, adm jr.
HAL3 CTL3 OSL  SL       0.00     3     0.00 ! methylsulfate
CTL2 OSL  SL   O2L      0.00     3     0.00 ! methylsulfate
CTL3 OSL  SL   O2L      0.00     3     0.00 ! methylsulfate
HEL1 CEL1 CEL1 HEL1     1.0000   2   180.00 ! 2-butene, adm jr., 8/98 update
CTL3 CEL1 CEL1 HEL1     1.0000   2   180.00 ! 2-butene, adm jr., 8/98 update
X    CEL1 CEL1 X        0.1300   1   180.00 ! 2-butene, adm jr., 8/98 update
X    CEL1 CEL1 X       24.0000   2   180.00 ! ethene, yin,adm jr., 12/95
X    CEL2 CEL2 X        4.9000   2   180.00 ! propene, yin,adm jr., 12/95
CTL2 CEL1 CEL2 HEL2     5.2000   2   180.00 ! propene, yin,adm jr., 12/95
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CTL3 CEL1 CEL2 HEL2      5.2000  2   180.00 ! propene, yin,adm jr., 12/95
HEL1 CEL1 CEL2 HEL2      5.2000  2   180.00 ! propene, yin,adm jr., 12/95
CEL1 CEL1 CTL2 HAL2      0.0300  3     0.00 ! butene, yin,adm jr., 12/95
CEL1 CEL1 CTL3 HAL3      0.0300  3     0.00 ! butene, yin,adm jr., 12/95
CEL1 CEL1 CTL2 CTL2      0.4000  3     0.00 ! 1-butene, adm jr., 8/98 update
CEL2 CEL1 CTL2 CTL2      0.4000  3     0.00 ! 1-butene, adm jr., 8/98 update
CEL2 CEL1 CTL2 CTL3      0.4000  3     0.00 ! 1-butene, adm jr., 8/98 update
CEL2 CEL1 CTL2 HAL2      0.1200  3     0.00 ! 1-butene, yin,adm jr., 12/95
CEL2 CEL1 CTL3 HAL3      0.050   3   180.00 ! propene, yin,adm jr., 12/95
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 CTL2 HAL2      0.8700  3     0.00 ! butene, yin,adm jr., 12/95
HEL1 CEL1 CTL3 HAL3      0.3400  3     0.00 ! butene, yin,adm jr., 12/95

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
!
OBL  X    X    CL         100.00    0      0.00 ! acetic acid
HEL2 HEL2 CEL2 CEL2        3.00    0      0.00 ! ethene, yin,adm jr., 12/95
OCL  X    X    CL          96.00    0      0.00 ! acetate

NONBONDED nbxmod  5 atom cdiel fshift vatom vdistance vfswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   eps,1-4       Rmin/2,1-4
!
HOL      0.0       -0.046     0.2245
HAL1     0.0       -0.022     1.3200 ! alkane, 3/92
HAL2     0.0       -0.028     1.3400 ! alkane, yin and mackerell, 4/98
HAL3     0.0       -0.024     1.3400 ! alkane, yin and mackerell, 4/98
HCL      0.0       -0.046     0.2245 ! ethanolamine
HT       0.0       -0.046     0.2245
HL       0.0       -0.046     0.7    ! polar H on NC4+
HEL1     0.0       -0.031     1.25   ! alkene, yin,adm jr., 12/95
HEL2     0.0       -0.026     1.26   ! alkene, yin,adm jr., 12/95
!
CL       0.0       -0.070     2.00   ! methyl acetate update
CTL1     0.0       -0.0200    2.275 0.0 -0.01 1.9 ! alkane, 3/92
CTL2     0.0       -0.0560    2.010 0.0 -0.01 1.9 ! alkane, 4/98, yin, adm jr.
CTL3     0.0       -0.0780    2.040 0.0 -0.01 1.9 ! alkane, 4/98, yin, adm jr.
CTL5     0.0       -0.0800    2.06  0.0 -0.01 1.9 ! old CTL3
                                                  ! maintained for tetramethylam
CEL1     0.0       -0.068     2.09   ! alkene, yin,adm jr., 12/95
CEL2     0.0       -0.064     2.08   ! alkene, yin,adm jr., 12/95
!
OBL      0.0       -0.12      1.70  0.0 -0.12 1.4
OCL      0.0       -0.12      1.70
O2L      0.0       -0.12      1.70
```

```
OHL      0.0        -0.1521    1.77
OSL      0.0        -0.1521    1.77
OT       0.0        -0.1521    1.7682
!
NH3L     0.0        -0.20      1.85   ! ethanolamine
NTL      0.0        -0.20      1.85   ! as all other nitogens
!
SL       0.0        -0.47      2.1    ! methylsulfate
PL       0.0        -0.585     2.15   ! ADM Jr.
DUM      0.0        -0.00      0.0    ! dummy atom
!
! ions, note lack of NBFIXes
!
SOD      0.0        -0.0469    1.36375    ! sodium
                    ! D. Beglovd and B. Roux, dA=-100.8 kcal/mol
POT      0.0        -0.0870    1.76375    ! potassium
                    ! D. Beglovd and B. Roux, dA=-82.36+2.8 = -79.56 kca/mol
CLA      0.0        -0.150      2.27      ! chloride
                    ! D. Beglovd and B. Roux, dA=-83.87+4.46 = -79.40 kcal/mol
MG       0.0        -0.0150    1.18500    ! Magnesium
                    ! B. Roux dA = -441.65

NBFIX
!                Emin         Rmin
!             (kcal/mol)      (A)
!

HBOND CUTHB 0.5  ! If you want to do hbond analysis (only), then use
                 ! READ PARAM APPEND CARD
                 ! to append hbond parameters from the file: par_hbond.inp

END
```