1 Supplementary Material: "Molecular Modeling and Simulations of AOT–water Reverse Micelles in Iso–octane: Structural and Dynamic Properties" by Stéphane Abel, Fabio Sterpone, Sanjoy Bandyopadhyay and Massimo Marchi

The following will provide potential parameters and topology for di–2–ethylhexylsulfoccinate, AOT and isooctane, as described in the paper. The actual files corresponding to the parameter and topology files of the program ORAC can be obtained from one of the authors (Massimo Marchi e–mail: `mmarchi@cea.fr`). These files can be easily adapted to run with other MD packages. For extensive information on the parameter and topology format of ORAC see its documentation on the web site `http://www.chim.unifi.it/orac/`.

1.1 Potential Parameters

The potential parameters given in this supplementary material refers to the potential function in Eq. 1 of the article, namely to:

$$\begin{aligned} V(\vec{R}) &= \sum_{stre.} k_b(b-b_0)^2 + \sum_{bend.} k_\theta(\theta-\theta_o)^2 \\ &+ \sum_{tors.} k_\phi(1+cos(n_\phi\phi+\delta)) + \sum_{impr.} k_\omega(\omega-\omega_o)^2 \\ &+ \sum_{i,j} 4\epsilon_{i,j}[(\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}] + \sum_{i,j}\frac{q_iq_j}{r_{ij}}. \end{aligned} \quad (1)$$

In the following parameter set, the units are used:

- Force constants ($K_b, K_\theta, K_\phi, K_\omega$) are in Kcal/mol
- Equilibrium distances (b_o) are in Å.
- Angles ($\theta_o, \delta, \omega_o$) are in degrees
- R^*_{ij} are in Å with $R^* = \sigma\sqrt[6]{2}$ with σ the Lennard–Jones diameter.
- ϵ_{ij} is in Kcal/mol.
- 1-4 interactions are scaled according to CHARMM's scaling factors: 1.0 for charge–charge interactions and 1.0 for Lennard–Jones.
- CHARMM's Berthelot mixing rules are used for all parameters.

In the following list, `BOND`, `BENDINGS`, `TORSION PROPER` and `TORSION IMPROPER` provide bond stretching, angle bending, torsion and improper torsion potential parameters. Following the keyword `NONBONDED MIXRULE` the Lennard–Jones parameters are given.

Parameter File

```
# \\\\\\\\\\\\\\ parameters for simulation of AOT\\\\\\\
#                   in decan solvent
#                    Taken from Charmm 27
#                  Translated to orac format
#\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
#
#                                  SOD
#
#                             OS1  OS2  OS3
#                              \    |   /
#                               \-- S--/              H21
#                                   |                 |
#                        O3=C3-------C1----------------C2-H21
#                           |        |                 |
#                          O2        H11               C12=O3
#                           |                          |
#                    H61 H41-C4-H42  H101              O4
#                     |      |        |                |
#               H62-C6-----C5--------C10-H102     H132-C13-H131      H151
#                     |      |        |                |             |
#                H72-C7-H71 H51 H112-C11-H111     H141-C14----------C15-H152
#                     |             |                |             |
#                H82-C8-H81          H113         H192-C19-H191 H162-C16-H161
#                     |                          |             |
#                H92-C9-H91                      H202 C20-H201 H172-C17-H171
#                     |                          |             |
#                    H93                            H203      H182-C18-H181
#                                                                |
#                                                               H183
################################
# BOND Unit: Kcal/mol-1 And angstroms
################################
#BONDS
#
#V(bond) = Kb(b - b0)**2
#
#Kb: kcal/mole/A**2
#b0: A
#
#atom type Kb          b0
BOND
ctl3 cl     200.00    1.522
ctl2 cl     200.00    1.522
ctl1 cl     200.00    1.522
obl  cl     750.00    1.220
ocl  cl     525.00    1.260
osl  cl     150.00    1.334
ohl  cl     230.00    1.400
hol  ohl    545.00    0.960
ctl1 hal1   309.00    1.111
ctl2 hal2   309.00    1.111
ctl3 hal3   322.00    1.111
ctl3 osl    340.00    1.430
ctl2 osl    340.00    1.430
ctl1 osl    340.00    1.430
osl  pl     270.00    1.600
o2l  pl     580.00    1.480
ohl  pl     237.00    1.590
nh3l hcl    410.00    1.040
nh3l ctl2   261.00    1.510
ntl  ctl2   215.00    1.510
ntl  ctl5   215.00    1.510
ctl5 hl     300.00    1.080
ctl2 hl     300.00    1.080
ctl1 ctl1   222.50    1.500
ctl1 ctl2   222.50    1.538
ctl1 ctl3   222.50    1.538
ctl2 ctl2   222.50    1.530
ctl2 ctl3   222.50    1.528
ctl3 ctl3   222.50    1.530
ohl  ctl1   428.00    1.420
ohl  ctl2   428.00    1.420
ohl  ctl3   428.00    1.420
sl   o2l    540.00    1.448
sl   osl    250.00    1.575
cel2 cel2   510.00    1.330
hel2 cel2   365.00    1.100
cel1 ctl3   383.00    1.504
cel1 cel2   500.00    1.342
hel1 cel1   360.50    1.100
cel1 ctl2   365.00    1.502
cel1 cel1   440.00    1.340
sl   ctl1   450.00    1.800
##############################
#
#For tetraedr carbon of isooctan
#
################################
ct0 ctl3  222.50    1.538
ct0 ctl2  222.50    1.538
```

```
##################
# isooctane and the aot
##################

ctl1   hal1   309.00     1.111
ctl2   hal2   309.00     1.111
ctl3   hal3   322.00     1.111
ctl1   ctl1   222.50     1.500
ctl1   ctl2   222.50     1.538
ctl1   ctl3   222.50     1.538
ctl2   ctl2   222.50     1.530
ctl2   ctl3   222.50     1.528


##################
#For TIP3P water model
##################

#ht     ht     0.0      1.5139
ht     ht    450.0      1.5139
ht     ot    450.0      0.9572
END
```

```
BENDINGS
obl  cl   ct13    70.00   125.00    20.00   2.44200
obl  cl   ct12    70.00   125.00    20.00   2.44200
obl  cl   ct11    70.00   125.00    20.00   2.44200
osl  cl   obl     90.00   125.90   160.00   2.25760
cl   osl  ct11    40.00   109.60    30.00   2.26510
cl   osl  ct12    40.00   109.60    30.00   2.26510
cl   osl  ct13    40.00   109.60    30.00   2.26510
hal2 ct12 cl      33.00   109.50    30.00   2.16300
hal3 ct13 cl      33.00   109.50    30.00   2.16300
ct12 ct12 cl      52.00   108.00
ct13 ct12 cl      52.00   108.00
ct12 ct11 cl      52.00   108.00
ct11 ct12 cl      52.00   108.00
osl  cl   ct13    55.00   109.00    20.00   2.32600
osl  cl   ct12    55.00   109.00    20.00   2.32600
ohl  cl   obl     50.00   123.00   210.00   2.26200
ocl  cl   ct12    40.00   118.00    50.00   2.38800
ocl  cl   ct13    40.00   118.00    50.00   2.38800
ocl  cl   ocl    100.00   124.00
ohl  cl   ct13    55.00   110.50
ohl  cl   ct12    55.00   110.50
hol  ohl  cl      55.00   115.00
osl  ct11 ct12    75.70   110.10
osl  ct11 ct13    75.70   110.10
osl  ct12 ct11    75.70   110.10
osl  ct12 ct12    75.70   110.10
osl  ct12 ct13    75.70   110.10
hal2 ct12 hal2    35.50   109.00     5.40   1.80200
hal3 ct13 hal3    35.50   108.40     5.40   1.80200
hal1 ct11 osl     60.00   109.50
hal2 ct12 osl     60.00   109.50
hal3 ct13 osl     60.00   109.50
ct12 osl  pl      20.00   120.00    35.00   2.33000
ct13 osl  pl      20.00   120.00    35.00   2.33000
hol  ohl  pl      30.00   115.00    40.00   2.30000
osl  pl   osl     80.00   104.30
osl  pl   o2l     98.90   111.60
osl  pl   ohl     48.10   108.00
o2l  pl   o2l    120.00   120.00
o2l  pl   ohl     98.90   108.23
nt1  ct12 hl      40.00   109.50    27.00   2.13000
nt1  ct15 hl      40.00   109.50    27.00   2.13000
hl   ct12 hl      24.00   109.50    28.00   1.76700
hl   ct15 hl      24.00   109.50    28.00   1.76700
ct15 nt1  ct12    60.00   109.50    26.00   2.46600
ct15 nt1  ct15    60.00   109.50    26.00   2.46600
hl   ct12 ct12    33.43   110.10    22.53   2.17900
hl   ct12 ct13    33.43   110.10    22.53   2.17900
hal1 ct11 ct11    34.50   110.10    22.53   2.17900
hal1 ct11 ct12    34.50   110.10    22.53   2.17900
hal1 ct11 ct13    34.50   110.10    22.53   2.17900
hal2 ct12 ct11    26.50   110.10    22.53   2.17900
hal2 ct12 ct12    26.50   110.10    22.53   2.17900

sl   ct11 hal1    34.50   110.10    22.53   2.17900
sl   ct11 cl      52.00   108.00
sl   ct11 ct12    58.35   113.50    11.16   2.56100
o2l  sl   o2l    130.00   109.47    35.00   2.45000
ct11 cl   osl     55.00   109.00    20.00   2.32600
o2l  sl   ct11    85.00    98.00
#########################################################

#############################
#
#For tetraedr carbon of isooctan
#
#############################
#############################################################
hal1 ct11 cl      33.000   109.50   30.00   2.16300
ct12 ct11 ct12    58.350   113.50   11.16   2.56100
ct11 ct12 ct13    58.350   113.50   11.16   2.56100
ct11 ct12 ct12    58.350   113.50   11.16   2.56100
ct13 ct0 ct13     58.350   113.50   11.16   2.56100
hal2 ct12 ct0     26.500   110.10   22.53   2.17900
ct13 ct0  ct12    58.350   113.50   11.16   2.56100
ct0  ct12 hal2    26.500   110.10   22.53   2.17900
hal3 ct13 ct0     33.430   110.10   22.53   2.17900
hal2 ct12 ct0     26.500   110.10   22.53   2.17900
ct0  ct12 ct11    58.350   113.50   11.16   2.56100
ct13 ct11 ct13    58.350   113.50   11.16   2.56100
#################
#
#################
hal3 ct13 hal3    35.500    109.00
hal2 ct12 hal2    26.500    110.10
hal2 ct12 ct13    34.600    110.10
hal2 ct12 ct12    26.500    110.10
ct13 ct12 ct12    58.000    115.00
hal3 ct13 ct12    34.600    110.10
ct12 ct12 ct12    58.350    113.60
hal2 ct12 ct13    34.600    110.10
```

```
ctl2 ctl3 hal3   34.600    110.10
hal3 ctl3 ctl1   33.430    110.10
ctl1 ctl3 hal3   33.430    110.10
ctl1 ctl2 ctl1   58.350    113.50
ctl2 ctl1 ctl3   58.350    113.50
ht   ot   ht     55.000    104.52
END
```

```
TORSION PROPER
x    ct11 oh1  x        0.1400   3       0.0
x    ct12 oh1  x        0.1400   3       0.0
x    ct13 oh1  x        0.1400   3       0.0
obl  cl   ct12 hal2     0.0000   6     180.0
obl  cl   ct13 hal3     0.0000   6     180.0
obl  cl   ct11 hal1     0.0000   6     180.0
osl  cl   ct12 hal2     0.0000   6     180.0
osl  cl   ct13 hal3     0.0000   6     180.0
osl  cl   ct11 hal1     0.0000   6     180.0
obl  cl   osl  ct11     0.9650   1     180.0
obl  cl   osl  ct11     3.8500   2     180.0
obl  cl   osl  ct12     0.9650   1     180.0
obl  cl   osl  ct12     3.8500   2     180.0
obl  cl   osl  ct13     0.9650   1     180.0
obl  cl   osl  ct13     3.8500   2     180.0
x    cl   osl  x        2.0500   2     180.0
x    ct12 cl   x        0.0500   6     180.0
x    ct13 cl   x        0.0500   6     180.0
x    ct11 cl   x        0.0500   6     180.0
x    cl   ohl  x        2.0500   2     180.0
hal2 ct12 cl   ohl      0.0000   6     180.0
hal3 ct13 cl   ohl      0.0000   6     180.0
osl  pl   osl  ct12     1.2000   1     180.0
osl  pl   osl  ct12     0.1000   2     180.0
osl  pl   osl  ct12     0.1000   3     180.0
o2l  pl   osl  ct12     0.1000   3       0.0
osl  pl   osl  ct13     1.2000   1     180.0
osl  pl   osl  ct13     0.1000   2     180.0
osl  pl   osl  ct13     0.1000   3     180.0
o2l  pl   osl  ct13     0.1000   3       0.0
ohl  pl   osl  ct12     0.9500   2       0.0
ohl  pl   osl  ct12     0.5000   3       0.0
ohl  pl   osl  ct13     0.9500   2       0.0
ohl  pl   osl  ct13     0.5000   3       0.0
x    ohl  pl   x        0.3000   3       0.0
x    ct11 osl  x        0.0000   3       0.0
x    ct12 osl  x        0.0000   3       0.0
x    ct13 osl  x        0.0000   3       0.0
ct13 ct12 osl  cl       0.7000   1     180.0
ct12 ct12 osl  cl       0.7000   1     180.0
ct13 ct11 osl  cl       0.7000   1     180.0
ct12 ct11 osl  cl       0.7000   1     180.0
ct11 ct12 osl  cl       0.7000   1     180.0
sl   ct11 ct12 cl       0.7000   1     180.0
ct11 ct12 cl   osl      0.1500   1     180.0
ct11 ct12 cl   osl      0.1500   1     180.0
ct11 ct12 cl   osl      0.5300   2     180.0
ct12 ct12 cl   osl      0.1500   1     180.0
ct12 ct12 cl   osl      0.1500   1     180.0
ct12 ct12 cl   osl      0.5300   2     180.0
ct12 ct11 cl   osl      0.1500   1     180.0
ct12 ct11 cl   osl      0.1500   1     180.0
ct12 ct11 cl   osl      0.5300   2     180.0
ct13 ct12 cl   osl      0.1500   1     180.0
ct13 ct12 cl   osl      0.1500   1     180.0
ct13 ct12 cl   osl      0.5300   2     180.0
sl   ct11 cl   osl      0.1500   1     180.0
sl   ct11 cl   osl      0.1500   1     180.0
sl   ct11 cl   osl      0.5300   2     180.0
x    ct12 nt1  x        0.2600   3       0.0
x    ct15 nt1  x        0.2300   3       0.0
x    ct12 nh3l x        0.1000   3       0.0
nh3l ct12 ct12 ohl      0.7000   1     180.0
nh3l ct12 ct12 osl      0.7000   1     180.0
nt1  ct12 ct12 ohl      4.3000   1     180.0
nt1  ct12 ct12 ohl      0.4000   3     180.0
nt1  ct12 ct12 ohl      0.4000   3     180.0
nt1  ct12 ct12 osl      3.3000   1     180.0
nt1  ct12 ct12 osl      0.4000   3     180.0
nt1  ct12 ct12 osl      0.4000   3     180.0
x    ct11 ct11 x        0.2000   3       0.0
x    ct11 ct12 x        0.2000   3       0.0
x    ct11 ct13 x        0.2000   3       0.0
hal3 ct13 osl  sl       0.0000   3       0.0
ct12 osl  sl   o2l      0.0000   3       0.0
ct13 osl  sl   o2l      0.0000   3       0.0
cl   ct11 sl   o2l      0.0000   3       0.0
hal1 ct11 sl   o2l      0.0000   3       0.0
ct12 ct11 sl   o2l      0.0000   3       0.0
hel1 cel1 cel1 hel1     1.0000   2     180.0
ct13 cel1 cel1 hel1     1.0000   2     180.0
x    cel1 cel1 x        0.1300   1     180.0
x    cel1 cel1 x       24.0000   2     180.0
x    cel2 cel2 x        4.9000   2     180.0
ct12 cel1 cel2 hel2     5.2000   2     180.0
ct13 cel1 cel2 hel2     5.2000   2     180.0
hel1 cel1 cel2 hel2     5.2000   2     180.0
cel1 cel1 ct12 hal2     0.0300   3       0.0
cel1 cel1 ct13 hal3     0.0300   3       0.0
cel1 cel1 ct12 ct12     0.4000   3       0.0
cel2 cel1 ct12 ct12     0.4000   3       0.0
```

```
cel2 cel1 ctl2 ctl3     0.4000   3       0.0
cel2 cel1 ctl2 hal2     0.1200   3       0.0
cel2 cel1 ctl3 hal3     0.0500   3     180.0
hel1 cel1 ctl2 ctl2     0.1200   3       0.0
hel1 cel1 ctl2 ctl3     0.1200   3       0.0
hel1 cel1 ctl2 hal2     0.8700   3       0.0
hel1 cel1 ctl3 hal3     0.3400   3       0.0
x    ct0 ctl3   x        0.200   3       0.0
x    ct0 ctl2   x        0.200   3       0.0
###################################
# For the isooctan and aot aot too
#
###################################
x    ctl2 ctl2 x         0.1900   3       0.0
x    ctl2 ctl3 x         0.1600   3       0.0
x    ctl3 ctl3 x         0.1525   3       0.0
ctl3 ctl2 ctl2 ctl3     0.1000   2     180.0
ctl3 ctl2 ctl2 ctl3     0.1500   4       0.0
ctl3 ctl2 ctl2 ctl3     0.1000   6     180.0
ctl2 ctl2 ctl2 ctl3     0.1000   2     180.0
ctl2 ctl2 ctl2 ctl3     0.1500   4       0.0
ctl2 ctl2 ctl2 ctl3     0.1000   6     180.0
ctl2 ctl2 ctl2 ctl2     0.1000   2     180.0
ctl2 ctl2 ctl2 ctl2     0.1500   4       0.0
ctl2 ctl2 ctl2 ctl2     0.1000   6     180.0
obl  x    x    cl     100.00    0.00000
hel2 hel2 cel2 cel2      3.00    0.00000
ocl  x    x    cl      96.00    0.00000
END
```

```
NONBONDED MIXRULE
##################
#For isooctan and aot molecule too
##################
#   s(all) e(all) s(14)  e(14) mass
hol      0.22450  -0.04600   0.00000   0.00000   1.00800
hcl      0.22450  -0.04600   0.00000   0.00000   1.00800
hl       0.70000  -0.04600   0.00000   0.00000   1.00800
hel1     1.25000  -0.03100   0.00000   0.00000   1.00800
hel2     1.26000  -0.02600   0.00000   0.00000   1.00800
cl       2.00000  -0.07000   0.00000   0.00000  12.01100
ctl1     2.27500  -0.02000   0.00000   0.00000  12.01100
############################################################
#  For decan and aot molecule
############################################################
hal1     1.32000  -0.02200   0.00000   0.00000   1.00800
hal2     1.34000  -0.02800   0.00000   0.00000   1.00800
hal3     1.34000  -0.02400   0.00000   0.00000   1.00800
ctl2     2.01000  -0.05600   0.00000   0.00000  12.01100
ctl3     2.04000  -0.07800   0.00000   0.00000  12.01100
############################################################
ctl5     2.06000  -0.08000   0.00000   0.00000  12.01100
cel1     2.09000  -0.06800   0.00000   0.00000  12.01100
cel2     2.08000  -0.06400   0.00000   0.00000  12.01100
obl      1.70000  -0.12000   0.00000   0.00000  15.99940
ocl      1.70000  -0.12000   0.00000   0.00000  15.99940
o2l      1.70000  -0.12000   0.00000   0.00000  15.99940
ohl      1.77000  -0.15210   0.00000   0.00000  15.99940
nh3l     1.85000  -0.20000   0.00000   0.00000  14.00700
ntl      1.85000  -0.20000   0.00000   0.00000  14.00700
sl       2.10000  -0.47000   0.00000   0.00000  32.06000
sod      1.36375  -0.04690   0.00000   0.00000  22.98977
osl      1.77000  -0.1521    0.00000   0.00000  15.99940
##############################
#
#For tetraedr carbon of isooctan
#
##############################
ct0      2.27500  -0.02000   0.00000   0.00000  12.01100
##############################
#  For the TiP3P water
##############################
ht       0.22450  -0.04600   0.00000   0.00000   1.00800
ot       1.76820  -0.15210   0.00000   0.00000  15.99940
##################################
END
```

1.2 Topology File

The following is the ORAC topology file AOT, residue `AOT`, and iso–octane, residue `ISO`. Charges are given as the third field within the keywords `atoms` and `group`, while labels and types are given as first and second fields. The keyword `bonds` contains a list of bonds each defined by two atom labels. The keyword `imphd` gives a list of improper torsions defined by four (4) labels. `termatom` is an ORAC internal keyword.

```
# \\\\\\\\\\\\\\ Topology for simulation of RM AOT \\\\\\\\
#                   in decan solvent
#                    Taken from Charmm 27
#                 Translated to orac format
#\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
#
#                                  SOD
#
#                             OS1  OS2  OS3
#                              \    |   /
#                               \-- S--/              H21
#                                    |                |
#                         O3=C3-------C1----------------C2-H21
#                             |       |                |
#                           O2        H11              C12=03
#                             |                        |
#                   H61 H41-C4-H42  H101               O4
#                     |      |        |                |
#               H62-C6-----C5--------C10-H102     H132-C13-H131      H151
#                     |      |        |                |             |
#                H72-C7-H71 H51 H112-C11-H111     H141-C14-----------C15-H152
#                     |             |                |             |
#                H82-C8-H81         H113          H192-C19-H191 H162-C16-H161
#                     |                              |             |
#                H92-C9-H91                        H202 C20-H201 H172-C17-H171
#                     |                              |             |
#                    H93                            H203      H182-C18-H181
#                                                                 |
#                                                                H183
#
##########################################
#
# For discard some pbs white Insight
# I use some code for each Hydrogens
#
# H1=H11, H2=H21, H3=H22, H4=H41, H5=H42, H6=H51
# H7=H51, H8=H62, H9=H71, H10=H72, H11=H81, H12=82
# H13=H91, H14=H92, H15=H93, H16=H101, H17=H102, H18=H111
# H19=H112, H20=H113, H21=H131, H22=H132, H23=H141, H24=H151
# H25=H152, H26=H161, H27=H162, H28=H171, H29=H172, H30=H181
# H31=H182, H32=H183, H33=H191, H34=H192, H35=201, H36=H202
# H37=H203 and SOD=Na
#
#
#



RESIDUE  AOT ( Total Charge =  -1.0 )
atoms
group
s       sl      1.3600
os1     o2l    -0.6000
os2     o2l    -0.6000
os3     o2l    -0.6000
c1      ct1l   -0.1900
h1      hal1    0.0900
group
c2      ct12   -0.1800
h2      hal2    0.0900
h3      hal2    0.0900
group
c3      cl      0.6300
o1      obl    -0.5200
o2      osl    -0.3400
group
c4      ct12   -0.1800
h4      hal2    0.0900
h5      hal2    0.0900
group
c5      ct1l   -0.0900
h6      hal1    0.0900
group
c6      ct12   -0.1800
h7      hal2    0.0900
h8      hal2    0.0900
group
c7      ct12   -0.1800
h9      hal2    0.0900
```

```
h10    hal2    0.0900
group
c8     ct12   -0.1800
h11    hal2    0.0900
h12    hal2    0.0900
group
c9     ct13   -0.2700
h13    hal3    0.0900
h14    hal3    0.0900
h15    hal3    0.0900
group
c10    ct12   -0.1800
h16    hal2    0.0900
h17    hal2    0.0900
group
c11    ct13   -0.2700
h18    hal3    0.0900
h19    hal3    0.0900
h20    hal3    0.0900
group
c12    cl      0.6300
o3     obl    -0.5200
o4     osl    -0.3400
group
c13    ct12   -0.1800
h21    hal2    0.0900
h22    hal2    0.0900
group
c14    ct11   -0.0900
h23    hal1    0.0900
group
c15    ct12   -0.1800
h24    hal2    0.0900
h25    hal2    0.0900
group
c16    ct12   -0.1800
h26    hal2    0.0900
h27    hal2    0.0900
group
c17    ct12   -0.1800
h28    hal2    0.0900
h29    hal2    0.0900
group
c18    ct13   -0.2700
h30    hal3    0.0900
h31    hal3    0.0900
h32    hal3    0.0900
group
c19    ct12   -0.1800
h33    hal2    0.0900
h34    hal2    0.0900
group
c20    ct13   -0.2700
h35    hal3    0.0900
h36    hal3    0.0900
h37    hal3    0.0900
#group
#na    sod      1.0000
end

bonds
s    os1    s    os2    s    os3
s    c1     c1   h1
c1   c3     c3   o1     c3   o2
o2   c4     c4   h4     c4   h5
c4   c5     c5   h6
c5   c6     c6   h7     c6   h8
c6   c7     c7   h9     c7   h10
c7   c8     c8   h11    c8   h12
c8   c9     c9   h13    c9   h14    c9   h15
c5   c10    c10  h16    c10  h17
c10  c11    c11  h18    c11  h19    c11  h20
c1   c2     c2   h2     c2   h3
c2   c12    c12  o3     c12  o4
o4   c13    c13  h21    c13  h22
c13  c14    c14  h23
c14  c15    c15  h24    c15  h25
c15  c16    c16  h26    c16  h27
c16  c17    c17  h28    c17  h29
c17  c18    c18  h30    c18  h31    c18  h32
c14  c19    c19  h33    c19  h34
c19  c20    c20  h35    c20  h36    c20  h37
end

imphd
o1   c1   o2   c3
o3   c2   o4   c12
end

termatom * *
RESIDUE_END
```

```
RESIDUE ISO ( Total Charge = 0.0)
atoms
group
c21 ct13   -0.2700
h38 hal3    0.0900
h39 hal3    0.0900
h40 hal3    0.0900
group
c22 ct0     0.0000
group
c23 ct12   -0.1800
h41 hal2    0.0900
h42 hal2    0.0900
group
c24 ct11   -0.0900
h43 hal1    0.0900
group
c25 ct13   -0.2700
h44 hal3    0.0900
h45 hal3    0.0900
h46 hal3    0.0900
# 3 methyl
group
c26 ct13   -0.2700
h47 hal3    0.0900
h48 hal3    0.0900
h49 hal3    0.0900
group
c27 ct13   -0.2700
h50 hal3    0.0900
h51 hal3    0.0900
h52 hal3    0.0900
group
c28 ct13   -0.2700
h53 hal3    0.0900
h54 hal3    0.0900
h55 hal3    0.0900
end

bonds

c21 c22  c22 c23  c23 c24
c24 c25  c22 c26  c22 c27
c24 c28
c21 h38  c21 h39  c21 h40
c23 h41  c23 h42
c24 h43
c25 h44  c25 h45  c25 h46
c26 h47  c26 h48  c26 h49
c27 h50  c27 h51  c27 h52
c28 h53  c28 h54  c28 h55
end

termatom * *
RESIDUE_END
```