* Topology Definition for CGenFF SAM Surface Residues
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* Mar 8, 2010
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! **
! Included below are the residues required for generating our alkanethiol SAM
! surfaces in CHARMM. The atom types and partial charges used here were
! obtained from the CHARMM General Force Field v. 2a5 for Small Molecule Drug
! Design, with a few exceptions that will be noted. CGenFF version 2a5 can be
! downloaded at:
! http://mackerell.umaryland.edu/CHARMM_ff_params.html
! The full citation for CGenFF is:
! Vanommeslaeghe K, Hatcher E, Acharya C, Kundu S, Zhong S, Shim J, Darian E,
! Guvench O, Lopes P, Vorobyov I, Mackerell AD Jr. CHARMM general force field:
! A force field for drug-like molecules compatible with the CHARMM all-atom
! additive biological force fields. J Comput Chem 31(4): 671-690 (2010).
!
! The SAM residues are all of the form H-S-(CH2)11-X and are given a three or
! four letter name determined by the functional group X:
!
! FUNCTIONAL GROUP: RESIDUE NAME:
! ---------------- -------------
! 1) -CH3   CH3
! 2) -OH   OHS
! 3) -COO-   COO
! 4) -COOH   COOH
! 5) -NH3+   NH3
! 6) -NH2   NH2
! 7) -COOCH3   COOC
! 8) -NHCOCH3   NHCO
! 9) -OC6H5   POXY
! 10) -OCH2CF3   TFCO
! 11) -(OCH2CH2)3OH PEGH
!
! To use these CGenFF residues with the CHARMM22 protein parameters, we included
! the following atom types in the "ATOM" section of the protein topology file.
!
! CHARMM CHARMM CHARMM MMFF ! DESCRIPTION OF CHARMM ATOMTYPE !! SAM RESIDUES
! index atom- mass atom- ! !! INCLUDING THIS
! type (in amu) type ! !! ATOM TYPE
! *** **********************
! MASS 225 CG321 12.01100 C ! aliphatic C for CH2 !! CH2
! MASS 226 HGA2 1.00800 H ! alphatic proton, CH2 !! CH2
! MASS 227 SG311 32.06000 S ! sulphur, SH, -S- !! SH
! MASS 228 HGP3 1.00800 H ! polar H, thiol !! SH

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! MASS  229 CG331   12.01100 C    ! aliphatic C for methyl group (-CH3)        !! CH3, COOC, NHCO
! MASS  230 HGA3     1.00800 H    ! alphatic proton, CH3                       !! CH3, COOC, NHCO
! MASS  231 OG311   15.99940 O    ! hydroxyl oxygen                            !! OH, COOH
! MASS  232 HGP1     1.00800 H    ! polar H                                    !! OH, COOH, NHCO, PEGH
! MASS  233 CG2O3   12.01100 C    ! carbonyl C: [negative] carboxylates        !! COO-
! MASS  234 OG2D2   15.99940 O    ! carbonyl O: negative groups: carboxylates,  !! COO-
!                        !                        carbonate      !!
! MASS  235 CG2O2   12.01100 C    ! carbonyl C: esters,                        !! COOH, COOC
!                        !           [neutral] carboxylic acids      !!
! MASS  236 OG2D1   15.99940 O    ! carbonyl O: amides, esters, aldehydes, urea !! COOH, COOC, NHCO
!                        !           [neutral] carboxylic acids      !!
! MASS  237 NG3P3   14.00700 N    ! primary NH3+, phosphatidylethanolamine     !! NH3+
! MASS  238 HGP2     1.00800 H    ! polar H, +ve charge                        !! NH3+
! MASS  239 CG324   12.01100 C    ! aliphatic C in CH2, adjacent to positive N  !! NH3+
!                        !                        (piperidine) (+) !!
! MASS  240 NG321   14.00700 N    ! neutral methylamine nitrogen               !! NH2
! MASS  241 HGPAM2   1.00800 H    ! polar H, NEUTRAL methylamine (#)           !! NH2
! MASS  242 OG302   15.99940 O    ! ester -O-                                  !! COOC
! MASS  243 CG2O1   12.01100 C    ! carbonyl C: amides                         !! NHCO
! MASS  244 NG2S1   14.00700 N    ! peptide nitrogen (CO=NHR)                  !! NHCO
! MASS  245 HGR61    1.00800 H    ! aromatic H                                 !! POXY
! MASS  246 CG2R61  12.01100 C    ! 6-mem aromatic C                           !! POXY
! MASS  247 OG301P  15.99940 O    ! ethoxybenzene ether -O- (~OG301 in CGenFF)  !! POXY
! MASS  248 OG301   15.99940 O    ! diethylether ether -O- (OG301 in CGenFF)    !! TFCO, PEGH
! MASS  249 CG302   12.01100 C    ! aliphatic C, no hydrogens, trifluoromethyl  !! TFCO
! MASS  250 FGA3    18.99800 F    ! aliphatic fluorine, trifluoro              !! TFCO
! MASS  251 OPEG    15.99940 O    ! hydroxyl oxygen for PEG (~OG311 in CGenFF)  !! PEGH
!
! Note that these atom types have been renumbered from the CGenFF topology and
! parameter files obtained at the Mackerell website so that they don't coincide
! with the CHARMM22 protein atom numbers.  We took the parameters from the
! CGenFF parameter file par_all36_cgenff.prm that corresponded to our SAM
! residues and supplemented them with our own parameters for the POXY, TFCO,
! and PEGH residues (listed in par_sams_cgenff.inp) to create a new parameter
! file just for the SAMs (all_sam_parameters.inp).  When running a simulation
! in CHARMM, the topology and parameter files were loaded using the following
! sequence:
!
!   READ rtf  card       NAME top_all22_prot.inp     <-- CGenFF ATOMs added
!   READ para card       NAME par_all22_prot.inp
!   READ rtf  card APPEND NAME top_sams_cgenff.inp
!   READ para card APPEND NAME all_sam_parameters.inp
!
! The internal coordinates (IC) defined for each neutral or cationic residue are
! those extracted from a MP2/6-31G(d) optimized geometry of a single functional-
! ized alkanethiol chain in vacuum.  A 6-31+G(d) basis set was used for the
! anionic COO- residue.  All of the MP2 infrared vibrational frequencies for
! each reported structure are real indicating energetically stable structures.
! These IC coordinates are only used in the initialization of the SAM geometry;
! the CHARMM force field characterizes the SAM structure during minimization
! and dynamics.
! ***************************************************************************
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DEFAult FIRSt NONE LAST NONE
AUTOgenerate ANGLes DIHEdral


! ***************************************************************************
! 01) -CH3 RESIDUE                                                          *
!                                                                           *
! SAM MODEL                          PARENT CGenFF RESIdue                  *
! *************************          *********************************
RESIdue    CH3    0.00 !                !
GROUp               !        H12C       ! Methyl from HEXA (hexane)
 ATOM  C12  CG331  -0.27 !       /         !
 ATOM  H12A HGA3    0.09 !  H12A-C12         !
 ATOM  H12B HGA3    0.09 !      / \          !
 ATOM  H12C HGA3    0.09 !    H12B  \        !
GROUp               !                !
 ATOM  C11  CG321  -0.18 !         C11-H11A   ! Methylene from HEXA (hexane)
 ATOM  H11A HGA2    0.09 !          / \       !
 ATOM  H11B HGA2    0.09 !         /  H11B    !
GROUp               !                !
 ATOM  C10  CG321  -0.18 !  H10A-C10          !
 ATOM  H10A HGA2    0.09 !      / \           !
 ATOM  H10B HGA2    0.09 !    H10B  \         !
GROUp               !                !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !          / \       !
 ATOM  H09B HGA2    0.09 !         /  H09B    !
GROUp               !                !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \           !
 ATOM  H08B HGA2    0.09 !    H08B  \         !
GROUp               !                !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !         /  H07B    !
GROUp               !                !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \           !
 ATOM  H06B HGA2    0.09 !    H06B  \         !
GROUp               !                !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !         /  H05B    !
GROUp               !                !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \           !
 ATOM  H04B HGA2    0.09 !    H04B  \         !
GROUp               !                !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !         /  H03B    !
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GROUp               !                 !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \           !
 ATOM  H02B HGA2    0.09 !    H02B  \         !
GROUp               !                 !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !        /   H01B    !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH            !
 ATOM  HS   HGP3    0.16 !       \            !
                !        HS        !
! ************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 C12   C11 H11A  C11 H11B
BOND     C12 H12C  C12 H12A  C12 H12B

!   i    j    k    l      R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5241    109.38    180.00   96.92   1.3418
IC   SH   C02  *C01 H01A    1.8242    109.38    120.41  109.81   1.0932
IC   SH   C02  *C01 H01B    1.8242    109.38   -120.41  109.81   1.0932
IC   SH   C01  C02  C03     1.8242    109.38    180.00  112.12   1.5283
IC   C01  C03  *C02 H02A    1.5241    112.12   -121.60  109.49   1.0973
IC   C01  C03  *C02 H02B    1.5241    112.12    121.60  109.49   1.0973
IC   C01  C02  C03  C04     1.5241    112.12    180.00  112.80   1.5274
IC   C02  C04  *C03 H03A    1.5283    112.80    121.93  109.25   1.0982
IC   C02  C04  *C03 H03B    1.5283    112.80   -121.93  109.25   1.0982
IC   C02  C03  C04  C05     1.5283    112.80    180.00  113.08   1.5270
IC   C03  C05  *C04 H04A    1.5274    113.08   -122.02  109.33   1.0986
IC   C03  C05  *C04 H04B    1.5274    113.08    122.02  109.33   1.0986
IC   C03  C04  C05  C06     1.5274    113.08    180.00  113.13   1.5277
IC   C04  C06  *C05 H05A    1.5270    113.13    122.05  109.28   1.0986
IC   C04  C06  *C05 H05B    1.5270    113.13   -122.05  109.28   1.0986
IC   C04  C05  C06  C07     1.5270    113.13    180.00  113.18   1.5273
IC   C05  C07  *C06 H06A    1.5277    113.18   -122.02  109.23   1.0980
IC   C05  C07  *C06 H06B    1.5277    113.18    122.02  109.23   1.0980
IC   C05  C06  C07  C08     1.5277    113.18    180.00  113.21   1.5271
IC   C06  C08  *C07 H07A    1.5273    113.21    122.08  109.21   1.0986
IC   C06  C08  *C07 H07B    1.5273    113.21   -122.08  109.21   1.0986
IC   C06  C07  C08  C09     1.5273    113.21    180.00  113.26   1.5276
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IC   C07  C09  *C08 H08A    1.5271    113.26   -122.08  109.23   1.0986
IC   C07  C09  *C08 H08B    1.5271    113.26    122.08  109.23   1.0986
IC   C07  C08  C09  C10     1.5271    113.26    180.00  113.24   1.5263
IC   C08  C10  *C09 H09A    1.5276    113.24    122.05  109.27   1.0986
IC   C08  C10  *C09 H09B    1.5276    113.24   -122.05  109.27   1.0986
IC   C08  C09  C10  C11     1.5276    113.24    180.00  113.33   1.5274
IC   C09  C11  *C10 H10A    1.5263    113.33   -122.10  109.18   1.0986
IC   C09  C11  *C10 H10B    1.5263    113.33    122.10  109.18   1.0986
IC   C09  C10  C11  C12     1.5263    113.33    180.00  112.84   1.5267
IC   C10  C12  *C11 H11A    1.5274    112.84    121.84  109.61   1.0972
IC   C10  C12  *C11 H11B    1.5274    112.84   -121.84  109.61   1.0972
IC   C10  C11  C12  H12C    1.5274    112.84    180.00  111.53   1.0941
IC   H12C C11  *C12 H12A    1.0941    111.53    120.21  110.86   1.0947
IC   H12C C11  *C12 H12B    1.0941    111.53   -120.21  110.86   1.0947
!    ------------------   ------- --------- --------- -------  -------

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! ***************************************************************************
! 02) -OH RESIDUE                                          *
!                                                          *
! SAM MODEL                              PARENT CGenFF RESIdue       *
! ************************               *********************************
RESIdue     OHS     0.00 !                 !
GROUp                !   HO - OH          ! Hydroxyl from SER (amino acid)
 ATOM  OH   OG311  -0.65 !        \          !       and ETAM (ethanolamine)
 ATOM  HO   HGP1    0.42 !        \         !
 ATOM  C11  CG321   0.05 !         C11-H11A   !
 ATOM  H11A HGA2    0.09 !          / \       !
 ATOM  H11B HGA2    0.09 !         /  H11B    !
GROUp                !                  !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \           !
 ATOM  H10B HGA2    0.09 !    H10B  \         !
GROUp                !                  !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !          / \       !
 ATOM  H09B HGA2    0.09 !         /  H09B    !
GROUp                !                  !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \           !
 ATOM  H08B HGA2    0.09 !    H08B  \         !
GROUp                !                  !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !         /  H07B    !
GROUp                !                  !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \           !
 ATOM  H06B HGA2    0.09 !    H06B  \         !
GROUp                !                  !
```

```
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !         /  H05B    !
GROUp               !                 !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \           !
 ATOM  H04B HGA2    0.09 !    H04B  \         !
GROUp               !                 !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !         /  H03B    !
GROUp               !                 !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \           !
 ATOM  H02B HGA2    0.09 !    H02B  \         !
GROUp               !                 !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !         /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH            !
 ATOM  HS   HGP3    0.16 !       \            !
                !        HS        !
! *************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 OH    C11 H11A  C11 H11B
BOND     OH  HO
DONOr    HO  OH
ACCEptor  OH

!   i    j    k    l     R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- ---------- -------  -------
IC   C02  C01  SH   HS     1.5240   109.32   -179.95   96.90   1.3414
IC   SH   C02  *C01 H01A   1.8249   109.32    120.31  109.89   1.0935
IC   SH   C02  *C01 H01B   1.8249   109.32   -120.35  109.85   1.0934
IC   SH   C01  C02  C03    1.8249   109.32   -179.95  112.06   1.5284
IC   C01  C03  *C02 H02A   1.5240   112.06   -121.56  109.47   1.0969
IC   C01  C03  *C02 H02B   1.5240   112.06    121.64  109.51   1.0966
IC   C01  C02  C03  C04    1.5240   112.06    179.97  112.79   1.5276
IC   C02  C04  *C03 H03A   1.5284   112.79    121.89  109.27   1.0983
IC   C02  C04  *C03 H03B   1.5284   112.79   -121.94  109.34   1.0978
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IC   C02  C03  C04  C05    1.5284   112.79  -179.95  113.07   1.5272
IC   C03  C05  *C04 H04A   1.5276   113.07  -121.96  109.31   1.0984
IC   C03  C05  *C04 H04B   1.5276   113.07   121.98  109.35   1.0980
IC   C03  C04  C05  C06    1.5276   113.07   179.96  113.15   1.5272
IC   C04  C06  *C05 H05A   1.5272   113.15   122.02  109.30   1.0986
IC   C04  C06  *C05 H05B   1.5272   113.15  -122.04  109.32   1.0990
IC   C04  C05  C06  C07    1.5272   113.15  -179.96  113.15   1.5272
IC   C05  C07  *C06 H06A   1.5272   113.15  -122.04  109.32   1.0982
IC   C05  C07  *C06 H06B   1.5272   113.15   122.01  109.29   1.0980
IC   C05  C06  C07  C08    1.5272   113.15   179.96  113.12   1.5278
IC   C06  C08  *C07 H07A   1.5272   113.12   121.96  109.25   1.0988
IC   C06  C08  *C07 H07B   1.5272   113.12  -122.06  109.27   1.0976
IC   C06  C07  C08  C09    1.5272   113.12  -179.92  113.12   1.5272
IC   C07  C09  *C08 H08A   1.5278   113.12  -122.01  109.30   1.0982
IC   C07  C09  *C08 H08B   1.5278   113.12   122.00  109.23   1.0982
IC   C07  C08  C09  C10    1.5278   113.12  -179.72  113.04   1.5268
IC   C08  C10  *C09 H09A   1.5272   113.04   122.08  109.58   1.0982
IC   C08  C10  *C09 H09B   1.5272   113.04  -121.79  109.27   1.0988
IC   C08  C09  C10  C11    1.5272   113.04  -179.63  112.83   1.5225
IC   C09  C11  *C10 H10A   1.5268   112.83  -121.78  109.04   1.0991
IC   C09  C11  *C10 H10B   1.5268   112.83   122.44  108.34   1.0966
IC   C09  C10  C11  OH     1.5268   112.83  -177.07  112.66   1.4289
IC   C10  OH   *C11 H11A   1.5225   112.66   124.08  110.99   1.0999
IC   C10  OH   *C11 H11B   1.5225   112.66  -120.04  105.16   1.0936
IC   C10  C11  OH   HO     1.5225   112.66   -62.56  106.93   0.9718
!   ------------------   ------- --------- --------- -------  -------

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! ****************************************************************************
! 03) -COO- RESIDUE                                                  *
!                                                                    *
! SAM MODEL                          PARENT CGenFF RESIdue       *
! *************************          *********************************
RESIdue    COO    -1.00 !     OD           ! Carboxylate
GROUp                !      \\           ! from GLU (amino acid)
 ATOM  C12  CG2O3   0.62 !       C12          !
 ATOM  OD   OG2D2  -0.76 !       / \          !
 ATOM  OH   OG2D2  -0.76 !  (-) OH   \         !
 ATOM  C11  CG321  -0.28 !         C11-H11A   !
 ATOM  H11A HGA2    0.09 !         / \        !
 ATOM  H11B HGA2    0.09 !        /  H11B     !
GROUp                !                  !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \          !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp                !                  !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !         / \        !
 ATOM  H09B HGA2    0.09 !        /  H09B     !
GROUp                !                  !
```

```
 ATOM  C08  CG321  -0.18 !  H08A-C08         !
 ATOM  H08A HGA2    0.09 !      / \          !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp               !                 !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !         / \       !
 ATOM  H07B HGA2    0.09 !        /  H07B    !
GROUp               !                 !
 ATOM  C06  CG321  -0.18 !  H06A-C06         !
 ATOM  H06A HGA2    0.09 !      / \          !
 ATOM  H06B HGA2    0.09 !    H06B  \        !
GROUp               !                 !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !         / \       !
 ATOM  H05B HGA2    0.09 !        /  H05B    !
GROUp               !                 !
 ATOM  C04  CG321  -0.18 !  H04A-C04         !
 ATOM  H04A HGA2    0.09 !      / \          !
 ATOM  H04B HGA2    0.09 !    H04B  \        !
GROUp               !                 !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !         / \       !
 ATOM  H03B HGA2    0.09 !        /  H03B    !
GROUp               !                 !
 ATOM  C02  CG321  -0.18 !  H02A-C02         !
 ATOM  H02A HGA2    0.09 !      / \          !
 ATOM  H02B HGA2    0.09 !    H02B  \        !
GROUp               !                 !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !         / \       !
 ATOM  H01B HGA2    0.09 !        /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH           !
 ATOM  HS   HGP3    0.16 !       \           !
                !        HS        !
! ************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 C12   C11 H11A  C11 H11B
BOND     C12 OH
DOUBLE    C12 OD
IMPRoper  C12 C11 OH  OD
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```
ACCEptor  OD  C12
ACCEptor  OH  C12

!   i    j    k    l     R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5236    109.53    179.05   96.97   1.3433
IC   SH   C02  *C01 H01A    1.8279    109.53    120.28  109.72   1.0949
IC   SH   C02  *C01 H01B    1.8279    109.53   -120.40  109.83   1.0942
IC   SH   C01  C02  C03     1.8279    109.53    179.89  111.91   1.5286
IC   C01  C03  *C02 H02A    1.5236    111.91   -121.60  109.44   1.0974
IC   C01  C03  *C02 H02B    1.5236    111.91    121.48  109.36   1.0985
IC   C01  C02  C03  C04     1.5236    111.91   -179.75  113.02   1.5279
IC   C02  C04  *C03 H03A    1.5286    113.02    121.89  109.15   1.0993
IC   C02  C04  *C03 H03B    1.5286    113.02   -122.00  109.17   1.0989
IC   C02  C03  C04  C05     1.5286    113.02   -179.73  113.09   1.5273
IC   C03  C05  *C04 H04A    1.5279    113.09   -121.93  109.26   1.0992
IC   C03  C05  *C04 H04B    1.5279    113.09    121.90  109.30   1.0988
IC   C03  C04  C05  C06     1.5279    113.09   -179.55  113.44   1.5278
IC   C04  C06  *C05 H05A    1.5273    113.44    122.10  109.17   1.1000
IC   C04  C06  *C05 H05B    1.5273    113.44   -122.05  109.16   1.0999
IC   C04  C05  C06  C07     1.5273    113.44   -179.61  113.32   1.5283
IC   C05  C07  *C06 H06A    1.5278    113.32   -121.99  109.17   1.0996
IC   C05  C07  *C06 H06B    1.5278    113.32    122.01  109.16   1.0994
IC   C05  C06  C07  C08     1.5278    113.32   -179.85  113.55   1.5274
IC   C06  C08  *C07 H07A    1.5283    113.55    122.05  109.17   1.1006
IC   C06  C08  *C07 H07B    1.5283    113.55   -122.04  109.17   1.0996
IC   C06  C07  C08  C09     1.5283    113.55   -179.48  113.54   1.5285
IC   C07  C09  *C08 H08A    1.5274    113.54   -122.08  109.10   1.1004
IC   C07  C09  *C08 H08B    1.5274    113.54    122.18  109.08   1.0995
IC   C07  C08  C09  C10     1.5274    113.54   -179.24  113.46   1.5288
IC   C08  C10  *C09 H09A    1.5285    113.46    122.15  109.52   1.1009
IC   C08  C10  *C09 H09B    1.5285    113.46   -121.87  109.07   1.1003
IC   C08  C09  C10  C11     1.5285    113.46   -179.62  113.58   1.5264
IC   C09  C11  *C10 H10A    1.5288    113.58   -121.89  108.95   1.1001
IC   C09  C11  *C10 H10B    1.5288    113.58    122.78  108.09   1.0966
IC   C09  C10  C11  C12     1.5288    113.58   -176.02  112.73   1.5547
IC   C10  C12  *C11 H11A    1.5264    112.73    123.42  108.94   1.0965
IC   C10  C12  *C11 H11B    1.5264    112.73   -120.19  107.59   1.1019
IC   C10  C11  C12  OD      1.5264    112.73   -134.64  116.14   1.2705
IC   OD   C11  *C12 OH      1.2705    116.14   -179.20  115.15   1.2714
!   -------------------   ------- --------- --------- -------  -------

PATChing FIRS NONE LAST NONE


! ***************************************************************************
! 04) -COOH RESIDUE                                          *
!                                                  *
! SAM MODEL                          PARENT CGenFF RESIdue       *
! ************************              ********************************
RESIdue    COOH    0.00 !                !
GROUp                 !     OD            ! Carboxyl
```

```
 ATOM  C12  CG2O2   0.75 !     \\           ! from GLUP (amino acid patch)
 ATOM  OD   OG2D1  -0.55 !  HO   C12         !
 ATOM  OH   OG311  -0.60 !   \ / \          !
 ATOM  HO   HGP1    0.43 !    OH   \        !
 ATOM  C11  CG321  -0.21 !         C11-H11A   !
 ATOM  H11A HGA2    0.09 !          / \       !
 ATOM  H11B HGA2    0.09 !         /  H11B    !
GROUp               !                !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \          !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp               !                !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !          / \       !
 ATOM  H09B HGA2    0.09 !         /  H09B    !
GROUp               !                !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \          !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp               !                !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !         /  H07B    !
GROUp               !                !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \          !
 ATOM  H06B HGA2    0.09 !    H06B  \        !
GROUp               !                !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !         /  H05B    !
GROUp               !                !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \          !
 ATOM  H04B HGA2    0.09 !    H04B  \        !
GROUp               !                !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !         /  H03B    !
GROUp               !                !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \          !
 ATOM  H02B HGA2    0.09 !    H02B  \        !
GROUp               !                !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !         /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH           !
 ATOM  HS   HGP3    0.16 !       \           !
                !        HS         !
! ************************                 *********************************
```

```
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 C12   C11 H11A  C11 H11B
BOND     C12 OH
DOUBLE    C12 OD
BOND     OH  HO
IMPRoper  C12 C11 OH  OD
DONOr     HO  OH
ACCEptor  OD  C12
ACCEptor  OH  C12

!   i    j    k    l      R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5235   109.35   179.95   96.89   1.3414
IC   SH   C02  *C01 H01A   1.8257   109.35   120.36  109.87   1.0936
IC   SH   C02  *C01 H01B   1.8257   109.35  -120.38  109.88   1.0936
IC   SH   C01  C02  C03    1.8257   109.35  -179.94  112.08   1.5281
IC   C01  C03  *C02 H02A   1.5235   112.08  -121.60  109.49   1.0967
IC   C01  C03  *C02 H02B   1.5235   112.08   121.64  109.49   1.0967
IC   C01  C02  C03  C04    1.5235   112.08  -179.93  112.81   1.5274
IC   C02  C04  *C03 H03A   1.5281   112.81   121.90  109.27   1.0984
IC   C02  C04  *C03 H03B   1.5281   112.81  -121.93  109.32   1.0983
IC   C02  C03  C04  C05    1.5281   112.81  -179.77  113.03   1.5278
IC   C03  C05  *C04 H04A   1.5274   113.03  -121.97  109.33   1.0977
IC   C03  C05  *C04 H04B   1.5274   113.03   121.97  109.35   1.0973
IC   C03  C04  C05  C06    1.5274   113.03  -179.86  113.12   1.5271
IC   C04  C06  *C05 H05A   1.5278   113.12   122.01  109.34   1.0985
IC   C04  C06  *C05 H05B   1.5278   113.12  -122.02  109.29   1.0986
IC   C04  C05  C06  C07    1.5278   113.12  -179.74  113.12   1.5279
IC   C05  C07  *C06 H06A   1.5271   113.12  -122.03  109.31   1.0980
IC   C05  C07  *C06 H06B   1.5271   113.12   122.01  109.26   1.0984
IC   C05  C06  C07  C08    1.5271   113.12  -179.84  113.18   1.5273
IC   C06  C08  *C07 H07A   1.5279   113.18   121.96  109.29   1.0993
IC   C06  C08  *C07 H07B   1.5279   113.18  -122.07  109.32   1.0981
IC   C06  C07  C08  C09    1.5279   113.18  -179.68  113.08   1.5272
IC   C07  C09  *C08 H08A   1.5273   113.08  -121.98  109.26   1.0981
IC   C07  C09  *C08 H08B   1.5273   113.08   122.03  109.35   1.0981
IC   C07  C08  C09  C10    1.5273   113.08  -179.76  112.82   1.5269
IC   C08  C10  *C09 H09A   1.5272   112.82   121.93  109.41   1.0980
IC   C08  C10  *C09 H09B   1.5272   112.82  -121.90  109.33   1.0982
IC   C08  C09  C10  C11    1.5272   112.82  -179.87  112.03   1.5334
IC   C09  C11  *C10 H10A   1.5269   112.03  -121.42  109.15   1.0978
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IC   C09  C11  *C10 H10B    1.5269    112.03    121.98  109.21   1.0955
IC   C09  C10  C11  C12     1.5269    112.03    178.32  111.76   1.5034
IC   C10  C12  *C11 H11A    1.5334    111.76    121.77  107.26   1.0926
IC   C10  C12  *C11 H11B    1.5334    111.76   -121.10  108.60   1.0955
IC   C10  C11  C12  OD      1.5334    111.76   -111.36  126.47   1.2192
IC   OD   C11  *C12 OH      1.2192    126.47    178.52  111.20   1.3650
IC   OD   C12  OH   HO      1.2192    122.32      0.24  105.39   0.9800
!    ------------------   ------- --------- --------- -------  -------

PATChing FIRS NONE LAST NONE


! ***************************************************************************
! 05) -NH3+ RESIDUE                                          *
!                                                 *
! SAM MODEL                           PARENT CGenFF RESIdue       *
! *************************           *********************************
RESIdue     NH3     1.00 !                  !
GROUp                !         HNC        ! Protonated amine
 ATOM  N    NG3P3  -0.30 !        /          ! from LYS (amino acid)
 ATOM  HNA  HGP2    0.33 !   HNA- N          !
 ATOM  HNB  HGP2    0.33 !      / \         !
 ATOM  HNC  HGP2    0.33 !    HNB  \        !
 ATOM  C11  CG324   0.21 !         C11-H11A   !
 ATOM  H11A HGA2    0.05 !          / \       !
 ATOM  H11B HGA2    0.05 !         /  H11B    !
GROUp                !                  !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \         !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp                !                  !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !          / \       !
 ATOM  H09B HGA2    0.09 !         /  H09B    !
GROUp                !                  !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \         !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp                !                  !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !         /  H07B    !
GROUp                !                  !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \         !
 ATOM  H06B HGA2    0.09 !    H06B  \        !
GROUp                !                  !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !         /  H05B    !
GROUp                !                  !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
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 ATOM  H04A HGA2    0.09 !      / \          !
 ATOM  H04B HGA2    0.09 !    H04B  \        !
GROUp                !                 !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !         /  H03B    !
GROUp                !                 !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \          !
 ATOM  H02B HGA2    0.09 !    H02B  \        !
GROUp                !                 !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \      !
 ATOM  H01B HGA2    0.09 !         /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH           !
 ATOM  HS   HGP3    0.16 !       \           !
                !        HS        !
! ************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 N     C11 H11A  C11 H11B
BOND     N   HNA   N   HNB   N   HNC
DONOr    HNA N
DONOr    HNB N
DONOr    HNC N

!   i    j    k    l      R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS      1.5247    109.11    180.00   96.83   1.3413
IC   SH   C02  *C01 H01A    1.8243    109.11    120.42  109.89   1.0939
IC   SH   C02  *C01 H01B    1.8243    109.11   -120.42  109.89   1.0939
IC   SH   C01  C02  C03     1.8243    109.11    180.00  112.23   1.5266
IC   C01  C03  *C02 H02A    1.5247    112.23   -121.59  109.58   1.0965
IC   C01  C03  *C02 H02B    1.5247    112.23    121.59  109.58   1.0965
IC   C01  C02  C03  C04     1.5247    112.23    180.00  112.59   1.5280
IC   C02  C04  *C03 H03A    1.5266    112.59    121.90  109.28   1.0982
IC   C02  C04  *C03 H03B    1.5266    112.59   -121.90  109.28   1.0982
IC   C02  C03  C04  C05     1.5266    112.59    180.00  113.08   1.5264
IC   C03  C05  *C04 H04A    1.5280    113.08   -121.95  109.36   1.0980
IC   C03  C05  *C04 H04B    1.5280    113.08    121.95  109.36   1.0980
IC   C03  C04  C05  C06     1.5280    113.08    180.00  112.89   1.5277
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```
IC   C04  C06  *C05 H05A    1.5264    112.89    121.97  109.33   1.0980
IC   C04  C06  *C05 H05B    1.5264    112.89   -121.97  109.33   1.0980
IC   C04  C05  C06  C07     1.5264    112.89    180.00  112.96   1.5276
IC   C05  C07  *C06 H06A    1.5277    112.96   -121.97  109.32   1.0980
IC   C05  C07  *C06 H06B    1.5277    112.96    121.97  109.32   1.0980
IC   C05  C06  C07  C08     1.5277    112.96    180.00  112.74   1.5281
IC   C06  C08  *C07 H07A    1.5276    112.74    121.86  109.36   1.0982
IC   C06  C08  *C07 H07B    1.5276    112.74   -121.86  109.36   1.0982
IC   C06  C07  C08  C09     1.5276    112.74    180.00  112.55   1.5286
IC   C07  C09  *C08 H08A    1.5281    112.55   -121.80  109.38   1.0976
IC   C07  C09  *C08 H08B    1.5281    112.55    121.80  109.38   1.0976
IC   C07  C08  C09  C10     1.5281    112.55    180.00  112.04   1.5314
IC   C08  C10  *C09 H09A    1.5286    112.04    121.55  109.49   1.0967
IC   C08  C10  *C09 H09B    1.5286    112.04   -121.55  109.49   1.0967
IC   C08  C09  C10  C11     1.5286    112.04    180.00  110.94   1.5169
IC   C09  C11  *C10 H10A    1.5314    110.94   -121.01  109.90   1.0981
IC   C09  C11  *C10 H10B    1.5314    110.94    121.01  109.90   1.0981
IC   C09  C10  C11  N       1.5314    110.94    180.00  110.37   1.5224
IC   C10  N    *C11 H11A    1.5169    110.37    122.01  106.18   1.0917
IC   C10  N    *C11 H11B    1.5169    110.37   -122.01  106.18   1.0917
IC   C10  C11  N    HNA     1.5169    110.37    -59.49  110.87   1.0285
IC   HNA  C11  *N   HNB     1.0285    110.87    118.98  110.87   1.0285
IC   HNA  C11  *N   HNC     1.0285    110.87   -120.51  112.43   1.0292
!    ------------------    -------  ---------  ---------  -------  -------

PATChing FIRS NONE LAST NONE


! ****************************************************************************
! 06) -NH2 RESIDUE                                                           *
!                                                                            *
! SAM MODEL                                PARENT CGenFF RESIdue             *
! ************************                 ***********************************
RESIdue     NH2     0.00 !                  !
GROUp                !                     ! Amine from
 ATOM  N    NG321  -0.96 !   HNA- N          ! PRES LSN (neutral LYS patch)
 ATOM  HNA  HGPAM2  0.34 !      / \          !
 ATOM  HNB  HGPAM2  0.34 !    HNB  \         !
 ATOM  C11  CG321   0.13 !         C11-H11A   !
 ATOM  H11A HGA2   0.075 !         / \        !
 ATOM  H11B HGA2   0.075 !        /  H11B     !
GROUp                !                     !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \          !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp                !                     !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !         / \        !
 ATOM  H09B HGA2    0.09 !        /  H09B     !
GROUp                !                     !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \          !
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 ATOM  H08B HGA2    0.09 !    H08B  \         !
GROUp               !                !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !         /  H07B    !
GROUp               !                !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \           !
 ATOM  H06B HGA2    0.09 !    H06B  \         !
GROUp               !                !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !         /  H05B    !
GROUp               !                !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \           !
 ATOM  H04B HGA2    0.09 !    H04B  \         !
GROUp               !                !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !         /  H03B    !
GROUp               !                !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \           !
 ATOM  H02B HGA2    0.09 !    H02B  \         !
GROUp               !                !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !         /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH            !
 ATOM  HS   HGP3    0.16 !       \            !
                !        HS         !
! ************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 N     C11 H11A  C11 H11B
BOND     N   HNA   N   HNB
DONOr    HNA N
DONOr    HNB N

!   i    j    k    l      R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
```

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!   ------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5242    109.42    180.00   96.86   1.3421
IC   SH   C02  *C01 H01A    1.8251    109.42    120.40  109.83   1.0932
IC   SH   C02  *C01 H01B    1.8251    109.42   -120.40  109.83   1.0932
IC   SH   C01  C02  C03     1.8251    109.42    180.00  112.08   1.5267
IC   C01  C03  *C02 H02A    1.5242    112.08   -121.58  109.53   1.0973
IC   C01  C03  *C02 H02B    1.5242    112.08    121.58  109.53   1.0973
IC   C01  C02  C03  C04     1.5242    112.08    180.00  112.81   1.5277
IC   C02  C04  *C03 H03A    1.5267    112.81   -121.97  109.27   1.0988
IC   C02  C04  *C03 H03B    1.5267    112.81    121.97  109.27   1.0988
IC   C02  C03  C04  C05     1.5267    112.81    180.00  113.10   1.5276
IC   C03  C05  *C04 H04A    1.5277    113.10   -121.99  109.30   1.0980
IC   C03  C05  *C04 H04B    1.5277    113.10    121.99  109.30   1.0980
IC   C03  C04  C05  C06     1.5277    113.10    180.00  113.16   1.5266
IC   C04  C06  *C05 H05A    1.5276    113.16    122.03  109.31   1.0986
IC   C04  C06  *C05 H05B    1.5276    113.16   -122.03  109.31   1.0986
IC   C04  C05  C06  C07     1.5276    113.16    180.00  113.16   1.5276
IC   C05  C07  *C06 H06A    1.5266    113.16   -122.05  109.27   1.0986
IC   C05  C07  *C06 H06B    1.5266    113.16    122.05  109.27   1.0986
IC   C05  C06  C07  C08     1.5266    113.16    180.00  113.18   1.5274
IC   C06  C08  *C07 H07A    1.5276    113.18    122.02  109.24   1.0980
IC   C06  C08  *C07 H07B    1.5276    113.18   -122.02  109.24   1.0980
IC   C06  C07  C08  C09     1.5276    113.18    180.00  113.18   1.5276
IC   C07  C09  *C08 H08A    1.5274    113.18   -122.05  109.27   1.0986
IC   C07  C09  *C08 H08B    1.5274    113.18    122.05  109.27   1.0986
IC   C07  C08  C09  C10     1.5274    113.18    180.00  113.23   1.5277
IC   C08  C10  *C09 H09A    1.5276    113.23    122.02  109.32   1.0986
IC   C08  C10  *C09 H09B    1.5276    113.23   -122.02  109.32   1.0986
IC   C08  C09  C10  C11     1.5276    113.23    180.00  113.16   1.5301
IC   C09  C11  *C10 H10A    1.5277    113.16   -122.11  109.00   1.0988
IC   C09  C11  *C10 H10B    1.5277    113.16    122.11  109.00   1.0988
IC   C09  C10  C11  N       1.5277    113.16    180.00  115.91   1.4658
IC   C10  N    *C11 H11A    1.5301    115.91    122.84  107.57   1.0961
IC   C10  N    *C11 H11B    1.5301    115.91   -122.84  107.57   1.0961
IC   C10  C11  N    HNA     1.5301    115.91    -57.53  109.15   1.0201
IC   C10  C11  N    HNB     1.5301    115.91     57.53  109.15   1.0201
!   ------------------   ------- --------- --------- -------  -------

PATChing FIRS NONE LAST NONE


! ****************************************************************************
! 07) -COOCH3 RESIDUE                                          *
!                                                              *
! SAM MODEL                          PARENT CGenFF RESIdue     *
! *************************          *********************************
RESIdue     COOC    0.00 !         H13C       !
GROUp                !        /          !
 ATOM  C13  CG331  -0.31 !  H13A-C13          ! Methoxycarbonyl from
 ATOM  H13A HGA3    0.09 !       / \          ! MBUT (methyl-butyrate)
 ATOM  H13B HGA3    0.09 !    H13B   OM       !
 ATOM  H13C HGA3    0.09 !         /          !
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 ATOM  OM   OG302  -0.49 !      C12          !
 ATOM  C12  CG2O2   0.90 !     // \         !
 ATOM  OD   OG2D1  -0.63 !    OD  \        !
 ATOM  C11  CG321   0.08 !         C11-H11A   !
 ATOM  H11A HGA2    0.09 !         / \       !
 ATOM  H11B HGA2    0.09 !        /  H11B    !
GROUp                !                !
 ATOM  C10  CG321  -0.18 !  H10A-C10          !
 ATOM  H10A HGA2    0.09 !      / \          !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp                !                !
 ATOM  C09  CG321  -0.18 !         C09-H09A   ! Methylene from HEXA (hexane)
 ATOM  H09A HGA2    0.09 !         / \       !
 ATOM  H09B HGA2    0.09 !        /  H09B    !
GROUp                !                !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \          !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp                !                !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !         / \       !
 ATOM  H07B HGA2    0.09 !        /  H07B    !
GROUp                !                !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \          !
 ATOM  H06B HGA2    0.09 !    H06B  \        !
GROUp                !                !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !         / \       !
 ATOM  H05B HGA2    0.09 !        /  H05B    !
GROUp                !                !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \          !
 ATOM  H04B HGA2    0.09 !    H04B  \        !
GROUp                !                !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !         / \       !
 ATOM  H03B HGA2    0.09 !        /  H03B    !
GROUp                !                !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \          !
 ATOM  H02B HGA2    0.09 !    H02B  \        !
GROUp                !                !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !         / \       !
 ATOM  H01B HGA2    0.09 !        /  H01B    !
                 !       /          !
 ATOM  SH   SG311  -0.23 !      SH           !
 ATOM  HS   HGP3    0.16 !       \          !
                 !        HS        !
! ************************                 *********************************
BOND     HS  SH
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```
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 C12   C11 H11A  C11 H11B
BOND     C12 OM
DOUBLE    C12 OD
BOND     OM  C13
BOND     C13 H13A  C13 H13B  C13 H13C
IMPRoper  C12 C11 OM  OD
ACCEptor  OM  C12
ACCEptor  OD  C12

!   i    j    k    l     R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5241    109.34    180.00   96.90   1.3418
IC   SH   C02  *C01 H01A    1.8254    109.34    120.38  109.88   1.0933
IC   SH   C02  *C01 H01B    1.8254    109.34   -120.38  109.88   1.0933
IC   SH   C01  C02  C03     1.8254    109.34    180.00  112.07   1.5277
IC   C01  C03  *C02 H02A    1.5241    112.07   -121.59  109.51   1.0972
IC   C01  C03  *C02 H02B    1.5241    112.07    121.59  109.51   1.0972
IC   C01  C02  C03  C04     1.5241    112.07    180.00  112.86   1.5269
IC   C02  C04  *C03 H03A    1.5277    112.86    121.97  109.26   1.0988
IC   C02  C04  *C03 H03B    1.5277    112.86   -121.97  109.26   1.0988
IC   C02  C03  C04  C05     1.5277    112.86    180.00  113.08   1.5274
IC   C03  C05  *C04 H04A    1.5269    113.08   -122.04  109.29   1.0986
IC   C03  C05  *C04 H04B    1.5269    113.08    122.04  109.29   1.0986
IC   C03  C04  C05  C06     1.5269    113.08    180.00  113.23   1.5277
IC   C04  C06  *C05 H05A    1.5274    113.23    122.06  109.25   1.0986
IC   C04  C06  *C05 H05B    1.5274    113.23   -122.06  109.25   1.0986
IC   C04  C05  C06  C07     1.5274    113.23    180.00  113.16   1.5263
IC   C05  C07  *C06 H06A    1.5277    113.16   -122.02  109.33   1.0986
IC   C05  C07  *C06 H06B    1.5277    113.16    122.02  109.33   1.0986
IC   C05  C06  C07  C08     1.5277    113.16    180.00  113.24   1.5275
IC   C06  C08  *C07 H07A    1.5263    113.24    122.06  109.26   1.0986
IC   C06  C08  *C07 H07B    1.5263    113.24   -122.06  109.26   1.0986
IC   C06  C07  C08  C09     1.5263    113.24    180.00  113.16   1.5265
IC   C07  C09  *C08 H08A    1.5275    113.16   -122.04  109.28   1.0986
IC   C07  C09  *C08 H08B    1.5275    113.16    122.04  109.28   1.0986
IC   C07  C08  C09  C10     1.5275    113.16    180.00  112.89   1.5274
IC   C08  C10  *C09 H09A    1.5265    112.89    121.93  109.49   1.0986
IC   C08  C10  *C09 H09B    1.5265    112.89   -121.93  109.49   1.0986
IC   C08  C09  C10  C11     1.5265    112.89    180.00  112.21   1.5231
IC   C09  C11  *C10 H10A    1.5274    112.21   -122.20  109.29   1.0955
IC   C09  C11  *C10 H10B    1.5274    112.21    122.20  109.29   1.0955
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IC   C09  C10  C11  C12    1.5274   112.21   180.00  112.71   1.5093
IC   C10  C12  *C11 H11A   1.5231   112.71   123.14  107.87   1.0967
IC   C10  C12  *C11 H11B   1.5231   112.71  -123.14  107.87   1.0967
IC   C10  C11  C12  OM     1.5231   112.71   180.00  110.73   1.3584
IC   OM   C11  *C12 OD     1.3584   110.73   180.00  125.88   1.2198
IC   C11  C12  OM   C13    1.5093   110.73   180.00  114.04   1.4414
IC   C12  OM   C13  H13A   1.3584   114.04   -60.46  110.45   1.0905
IC   H13A OM   *C13 H13B   1.0905   110.45   120.93  110.45   1.0905
IC   H13A OM   *C13 H13C   1.0905   110.45  -119.54  105.05   1.0883
!    ------------------   ------- --------- --------- -------  -------

PATChing FIRS NONE LAST NONE


! ***************************************************************************
! 08) -NHCOCH3 RESIDUE                                          *
!                                                 *
! SAM MODEL                              PARENT CGenFF RESIdue       *
! ************************                 *********************************
RESIdue     NHCO    0.00 !                  !
GROUp                !        H13C        ! -CO-CH3 charge groups
 ATOM  C13  CG331  -0.27 !       /           ! from NMA (N-methylacetamide)
 ATOM  H13A HGA3    0.09 ! H13A-C13           !
 ATOM  H13B HGA3    0.09 !     / \           !
 ATOM  H13C HGA3    0.09 !   H13B  \         !
GROUp                !        C12         !
 ATOM  C12  CG2O1   0.51 !       || \  HN     !
 ATOM  OD   OG2D1  -0.51 !       OD  \ |      !
GROUP                !           N        ! -NH-CH2- charge group
 ATOM  N    NG2S1  -0.47 !            \       ! from GLY (amino acid)
 ATOM  HN   HGP1    0.31 !             \     !
 ATOM  C11  CG321  -0.02 !            C11-H11A!
 ATOM  H11A HGA2    0.09 !              / \    !
 ATOM  H11B HGA2    0.09 !             /  H11B  !
GROUp                !                  !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \          !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp                !                  !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !          / \       !
 ATOM  H09B HGA2    0.09 !         /  H09B    !
GROUp                !                  !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \          !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp                !                  !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !         /  H07B    !
GROUp                !                  !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
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```
 ATOM  H06A HGA2    0.09 !      / \         !
 ATOM  H06B HGA2    0.09 !    H06B  \       !
GROUp               !                !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !         /  H05B    !
GROUp               !                !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \         !
 ATOM  H04B HGA2    0.09 !    H04B  \       !
GROUp               !                !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !         /  H03B    !
GROUp               !                !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \         !
 ATOM  H02B HGA2    0.09 !    H02B  \       !
GROUp               !                !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !         /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH           !
 ATOM  HS   HGP3    0.16 !       \           !
                !        HS        !
! *************************                 *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 N     C11 H11A  C11 H11B
BOND     N   C12   N   HN
BOND     C12 C13
DOUBLE    C12 OD
BOND     C13 H13A  C13 H13B  C13 H13C
IMPRoper  N   C12  C11 HN
IMPRoper  C12 C13  N   OD
DONOr     HN  N
ACCEptor  OD  C12

!   i    j    k    l      R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS      1.5251    109.35   -179.86   96.89   1.3415
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```
IC   SH   C02  *C01 H01A    1.8251    109.35    120.41  109.87   1.0933
IC   SH   C02  *C01 H01B    1.8251    109.35   -120.35  109.82   1.0931
IC   SH   C01  C02  C03     1.8251    109.35   -179.81  112.07   1.5278
IC   C01  C03  *C02 H02A    1.5251    112.07   -121.52  109.54   1.0969
IC   C01  C03  *C02 H02B    1.5251    112.07    121.60  109.58   1.0961
IC   C01  C02  C03  C04     1.5251    112.07   -179.95  112.79   1.5273
IC   C02  C04  *C03 H03A    1.5278    112.79    121.91  109.29   1.0980
IC   C02  C04  *C03 H03B    1.5278    112.79   -121.94  109.30   1.0979
IC   C02  C03  C04  C05     1.5278    112.79   -179.69  113.13   1.5268
IC   C03  C05  *C04 H04A    1.5273    113.13   -121.92  109.30   1.0992
IC   C03  C05  *C04 H04B    1.5273    113.13    122.04  109.36   1.0978
IC   C03  C04  C05  C06     1.5273    113.13   -179.97  113.14   1.5270
IC   C04  C06  *C05 H05A    1.5268    113.14    122.04  109.32   1.0982
IC   C04  C06  *C05 H05B    1.5268    113.14   -122.03  109.27   1.0992
IC   C04  C05  C06  C07     1.5268    113.14   -179.73  113.20   1.5274
IC   C05  C07  *C06 H06A    1.5270    113.20   -122.01  109.27   1.0984
IC   C05  C07  *C06 H06B    1.5270    113.20    122.06  109.26   1.0977
IC   C05  C06  C07  C08     1.5270    113.20   -179.98  113.18   1.5274
IC   C06  C08  *C07 H07A    1.5274    113.18    122.04  109.27   1.0989
IC   C06  C08  *C07 H07B    1.5274    113.18   -122.07  109.24   1.0985
IC   C06  C07  C08  C09     1.5274    113.18   -179.82  113.20   1.5272
IC   C07  C09  *C08 H08A    1.5274    113.20   -122.03  109.31   1.0987
IC   C07  C09  *C08 H08B    1.5274    113.20    121.99  109.18   1.0985
IC   C07  C08  C09  C10     1.5274    113.20   -179.68  112.90   1.5271
IC   C08  C10  *C09 H09A    1.5272    112.90    122.07  109.62   1.0983
IC   C08  C10  *C09 H09B    1.5272    112.90   -121.72  109.19   1.0986
IC   C08  C09  C10  C11     1.5272    112.90    179.48  112.30   1.5267
IC   C09  C11  *C10 H10A    1.5271    112.30   -122.20  109.34   1.0973
IC   C09  C11  *C10 H10B    1.5271    112.30    121.39  108.02   1.0961
IC   C09  C10  C11  N       1.5271    112.30   -179.33  113.09   1.4552
IC   C10  N    *C11 H11A    1.5267    113.09    122.90  107.98   1.0956
IC   C10  N    *C11 H11B    1.5267    113.09   -121.10  107.06   1.0931
IC   C10  C11  N    C12     1.5267    113.09     79.50  120.73   1.3665
IC   C11  C12  *N   HN      1.4552    120.73    165.38  118.92   1.0112
IC   HN   N    C12  C13     1.0112    118.92    -12.43  115.47   1.5162
IC   N    C13  *C12 OD      1.3665    115.47    176.72  122.23   1.2341
IC   N    C12  C13  H13A    1.3665    115.47     24.56  113.02   1.0933
IC   N    C12  C13  H13B    1.3665    115.47    146.23  108.48   1.0901
IC   N    C12  C13  H13C    1.3665    115.47    -96.29  109.05   1.0938
!    ------------------   ------- --------- --------- -------  -------

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! ***************************************************************************
! 09) -OC6H5 RESIDUE                                        *
!                                                           *
! SAM MODEL                          PARENT CGenFF RESIdue       *
! ************************           *********************************
RESIdue    POXY     0.00 !                 !
GROUp                 !                  !
 ATOM C17  CG2R61 -0.115 !                  ! Phenoxy charge groups
```

```
 ATOM H17  HGR61   0.115 !                 ! from ETOB (ethoxybenzene)
GROUp                !         H17       !
 ATOM C16  CG2R61 -0.115 !          |       !
 ATOM H16  HGR61   0.115 !         C17      !
GROUp                !        /   \      !
 ATOM C15  CG2R61 -0.115 !    H15-C15   C16-H16 !
 ATOM H15  HGR61   0.115 !       |    |     !
GROUp                !       |    |     !
 ATOM C14  CG2R61 -0.115 !    H13-C13   C14-H14 !
 ATOM H14  HGR61   0.115 !        \  /      !
GROUp                !         C12       !
 ATOM C13  CG2R61 -0.115 !         /        !
 ATOM H13  HGR61   0.115 !        /         !
GROUp                !        O          !
 ATOM C12  CG2R61   0.22 !         \         !
 ATOM O    OG301P  -0.39 !          \        !
 ATOM C11  CG321   -0.01 !          C11-H11A   !
 ATOM H11A HGA2     0.09 !           / \       !
 ATOM H11B HGA2     0.09 !          /  H11B    !
GROUp                !                  !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \          !
 ATOM  H10B HGA2    0.09 !    H10B  \        !
GROUp                !                  !
 ATOM  C09  CG321  -0.18 !          C09-H09A   !
 ATOM  H09A HGA2    0.09 !           / \       !
 ATOM  H09B HGA2    0.09 !          /  H09B    !
GROUp                !                  !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \          !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp                !                  !
 ATOM  C07  CG321  -0.18 !          C07-H07A   !
 ATOM  H07A HGA2    0.09 !           / \       !
 ATOM  H07B HGA2    0.09 !          /  H07B    !
GROUp                !                  !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \          !
 ATOM  H06B HGA2    0.09 !    H06B  \        !
GROUp                !                  !
 ATOM  C05  CG321  -0.18 !          C05-H05A   !
 ATOM  H05A HGA2    0.09 !           / \       !
 ATOM  H05B HGA2    0.09 !          /  H05B    !
GROUp                !                  !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \          !
 ATOM  H04B HGA2    0.09 !    H04B  \        !
GROUp                !                  !
 ATOM  C03  CG321  -0.18 !          C03-H03A   !
 ATOM  H03A HGA2    0.09 !           / \       !
 ATOM  H03B HGA2    0.09 !          /  H03B    !
GROUp                !                  !
```

```
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \           !
 ATOM  H02B HGA2    0.09 !    H02B  \         !
GROUp                 !                  !
 ATOM  C01  CG321  -0.11 !          C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !        /   H01B    !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH            !
 ATOM  HS   HGP3    0.16 !       \            !
                !        HS        !
! ************************                ********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 O     C11 H11A  C11 H11B
BOND     O   C12
BOND     C12 C13   C12 C14
BOND     C13 H13   C13 C15
BOND     C14 H14   C14 C16
BOND     C15 H15   C15 C17
BOND     C16 H16   C16 C17
BOND     C17 H17

!   i    j    k    l      R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5242    109.34    180.00   96.90   1.3418
IC   SH   C02  *C01 H01A   1.8245    109.34    120.39  109.86   1.0933
IC   SH   C02  *C01 H01B   1.8245    109.34   -120.39  109.86   1.0933
IC   SH   C01  C02  C03    1.8245    109.34    180.00  112.08   1.5278
IC   C01  C03  *C02 H02A   1.5242    112.08   -121.56  109.53   1.0971
IC   C01  C03  *C02 H02B   1.5242    112.08    121.56  109.53   1.0971
IC   C01  C02  C03  C04    1.5242    112.08    180.00  112.82   1.5273
IC   C02  C04  *C03 H03A   1.5278    112.82    121.95  109.25   1.0985
IC   C02  C04  *C03 H03B   1.5278    112.82   -121.95  109.25   1.0985
IC   C02  C03  C04  C05    1.5278    112.82    180.00  113.07   1.5272
IC   C03  C05  *C04 H04A   1.5273    113.07   -122.00  109.33   1.0983
IC   C03  C05  *C04 H04B   1.5273    113.07    122.00  109.33   1.0983
IC   C03  C04  C05  C06    1.5273    113.07    180.00  113.18   1.5263
IC   C04  C06  *C05 H05A   1.5272    113.18    122.06  109.30   1.0989
IC   C04  C06  *C05 H05B   1.5272    113.18   -122.06  109.30   1.0989
IC   C04  C05  C06  C07    1.5272    113.18    180.00  113.18   1.5272
IC   C05  C07  *C06 H06A   1.5263    113.18   -122.08  109.25   1.0989
```

```
IC   C05  C07  *C06 H06B    1.5263    113.18    122.08  109.25   1.0989
IC   C05  C06  C07  C08     1.5263    113.18    180.00  113.20   1.5271
IC   C06  C08  *C07 H07A    1.5272    113.20    122.07  109.28   1.0989
IC   C06  C08  *C07 H07B    1.5272    113.20   -122.07  109.28   1.0989
IC   C06  C07  C08  C09     1.5272    113.20    180.00  113.07   1.5270
IC   C07  C09  *C08 H08A    1.5271    113.07   -122.03  109.26   1.0983
IC   C07  C09  *C08 H08B    1.5271    113.07    122.03  109.26   1.0983
IC   C07  C08  C09  C10     1.5271    113.07    180.00  112.71   1.5278
IC   C08  C10  *C09 H09A    1.5270    112.71    121.84  109.59   1.0982
IC   C08  C10  *C09 H09B    1.5270    112.71   -121.84  109.59   1.0982
IC   C08  C09  C10  C11     1.5270    112.71    180.00  112.16   1.5162
IC   C09  C11  *C10 H10A    1.5278    112.16   -121.97  108.55   1.0954
IC   C09  C11  *C10 H10B    1.5278    112.16    121.97  108.55   1.0954
IC   C09  C10  C11  O       1.5278    112.16    180.00  107.10   1.4296
IC   C10  O    *C11 H11A    1.5162    107.10    120.47  110.10   1.0996
IC   C10  O    *C11 H11B    1.5162    107.10   -120.47  110.10   1.0996
IC   C10  C11  O    C12     1.5162    107.10    180.00  117.26   1.3721
IC   C11  O    C12  C13     1.4296    117.26    180.00  115.11   1.4022
IC   C13  O    *C12 C14     1.4022    115.11    180.00  124.86   1.3998
IC   O    C12  C13  C15     1.3721    115.11    180.00  120.03   1.3901
IC   C15  C12  *C13 H13     1.3901    120.03    180.00  118.28   1.0867
IC   O    C12  C14  C16     1.3721    124.86    180.00  119.22   1.3996
IC   C16  C12  *C14 H14     1.3996    119.22    180.00  121.30   1.0847
IC   C12  C13  C15  C17     1.4022    120.03      0.00  120.41   1.3995
IC   C17  C13  *C15 H15     1.3995    120.41    180.00  119.43   1.0878
IC   C17  C14  *C16 H16     1.3925    120.98    180.00  118.96   1.0875
IC   C15  C16  *C17 H17     1.3995    119.32    180.00  120.30   1.0870
!    ------------------    -------  ---------  ---------  -------  -------

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! ***************************************************************************
! 10) -OCH2CF3 RESIDUE                                          *
!                                                               *
! SAM MODEL                          PARENT CGenFF RESIdue      *
! ************************           *********************************
RESIdue     TFCO    0.00 !          FB   FC  !
                    !              \ /    ! Trifluoroethoxy charge group
GROUp               !              C13    ! was manufactured by combining
 ATOM  C13  CG302   0.34 !        H12B  / \    ! the -CH2-CF3 from TFE
 ATOM  FA   FGA3   -0.14 !          \ /    FA  ! (trifluoroethanol) with the
 ATOM  FB   FGA3   -0.14 !          C12        ! -CH2-O-CH2- from DETE
 ATOM  FC   FGA3   -0.14 !         / \         ! (diethylether) with a charge
 ATOM  C12  CG321   0.07 !        /   H12A     ! of -0.01 added to O and a
 ATOM  H12A HGA2    0.09 !       O            ! charge of +0.09 added to C12
 ATOM  H12B HGA2    0.09 !        \           ! due to the Fluorines pulling
 ATOM  O    OG301  -0.34 !         \          ! extra electron density toward
 ATOM  C11  CG321  -0.01 !          C11-H11A   ! them.
 ATOM  H11A HGA2    0.09 !           / \       !
 ATOM  H11B HGA2    0.09 !          /  H11B    !
GROUp               !              !
```

```
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \           !
 ATOM  H10B HGA2    0.09 !    H10B  \         !
GROUp                 !                  !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !          / \       !
 ATOM  H09B HGA2    0.09 !        /  H09B     !
GROUp                 !                  !
 ATOM  C08  CG321  -0.18 !  H08A-C08          !
 ATOM  H08A HGA2    0.09 !      / \           !
 ATOM  H08B HGA2    0.09 !    H08B  \         !
GROUp                 !                  !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !          / \       !
 ATOM  H07B HGA2    0.09 !        /  H07B     !
GROUp                 !                  !
 ATOM  C06  CG321  -0.18 !  H06A-C06          !
 ATOM  H06A HGA2    0.09 !      / \           !
 ATOM  H06B HGA2    0.09 !    H06B  \         !
GROUp                 !                  !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !          / \       !
 ATOM  H05B HGA2    0.09 !        /  H05B     !
GROUp                 !                  !
 ATOM  C04  CG321  -0.18 !  H04A-C04          !
 ATOM  H04A HGA2    0.09 !      / \           !
 ATOM  H04B HGA2    0.09 !    H04B  \         !
GROUp                 !                  !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !          / \       !
 ATOM  H03B HGA2    0.09 !        /  H03B     !
GROUp                 !                  !
 ATOM  C02  CG321  -0.18 !  H02A-C02          !
 ATOM  H02A HGA2    0.09 !      / \           !
 ATOM  H02B HGA2    0.09 !    H02B  \         !
GROUp                 !                  !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !          / \       !
 ATOM  H01B HGA2    0.09 !        /   H01B    !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH            !
 ATOM  HS   HGP3    0.16 !       \            !
                !        HS         !
! ************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
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```
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 O     C11 H11A  C11 H11B
BOND     O   C12
BOND     C12 C13   C12 H12A  C12 H12B
BOND     C13 FA    C13 FB    C13 FC

!   i    j    k    l     R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   -------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5238    109.36    179.94   96.88   1.3418
IC   SH   C02  *C01 H01A    1.8253    109.36    120.43  109.94   1.0939
IC   SH   C02  *C01 H01B    1.8253    109.36   -120.38  109.88   1.0936
IC   SH   C01  C02  C03     1.8253    109.36    179.91  112.05   1.5275
IC   C01  C03  *C02 H02A    1.5238    112.05   -121.55  109.54   1.0969
IC   C01  C03  *C02 H02B    1.5238    112.05    121.61  109.54   1.0958
IC   C01  C02  C03  C04     1.5238    112.05    179.99  112.78   1.5278
IC   C02  C04  *C03 H03A    1.5275    112.78    121.99  109.26   1.0979
IC   C02  C04  *C03 H03B    1.5275    112.78   -121.90  109.24   1.0977
IC   C02  C03  C04  C05     1.5275    112.78    179.93  113.11   1.5271
IC   C03  C05  *C04 H04A    1.5278    113.11   -121.99  109.32   1.0979
IC   C03  C05  *C04 H04B    1.5278    113.11    122.04  109.36   1.0986
IC   C03  C04  C05  C06     1.5278    113.11    179.99  113.13   1.5273
IC   C04  C06  *C05 H05A    1.5271    113.13    122.05  109.30   1.0985
IC   C04  C06  *C05 H05B    1.5271    113.13   -121.99  109.30   1.0989
IC   C04  C05  C06  C07     1.5271    113.13   -180.00  113.15   1.5280
IC   C05  C07  *C06 H06A    1.5273    113.15   -122.03  109.26   1.0979
IC   C05  C07  *C06 H06B    1.5273    113.15    122.01  109.28   1.0990
IC   C05  C06  C07  C08     1.5273    113.15    179.83  113.11   1.5266
IC   C06  C08  *C07 H07A    1.5280    113.11    121.96  109.32   1.0987
IC   C06  C08  *C07 H07B    1.5280    113.11   -122.01  109.36   1.0984
IC   C06  C07  C08  C09     1.5280    113.11   -179.86  113.08   1.5283
IC   C07  C09  *C08 H08A    1.5266    113.08   -122.01  109.24   1.0977
IC   C07  C09  *C08 H08B    1.5266    113.08    122.06  109.24   1.0982
IC   C07  C08  C09  C10     1.5266    113.08    179.70  112.72   1.5274
IC   C08  C10  *C09 H09A    1.5283    112.72    121.73  109.53   1.0978
IC   C08  C10  *C09 H09B    1.5283    112.72   -121.86  109.68   1.0978
IC   C08  C09  C10  C11     1.5283    112.72   -179.64  112.21   1.5149
IC   C09  C11  *C10 H10A    1.5274    112.21   -121.76  108.39   1.0960
IC   C09  C11  *C10 H10B    1.5274    112.21    122.30  108.75   1.0953
IC   C09  C10  C11  O       1.5274    112.21    178.34  107.28   1.4354
IC   C10  O    *C11 H11A    1.5149    107.28    120.93  110.57   1.0957
IC   C10  O    *C11 H11B    1.5149    107.28   -120.42  109.52   1.1014
IC   C10  C11  O    C12     1.5149    107.28    163.25  114.80   1.4051
IC   C11  O    C12  C13     1.4354    114.80     78.68  113.04   1.5141
IC   C13  O    *C12 H12A    1.5141    113.04   -122.29  112.63   1.0995
IC   H12A O    *C12 H12B    1.0995    112.63   -120.02  107.26   1.0927
IC   O    C12  C13  FA      1.4051    113.04    -67.92  112.31   1.3559
IC   O    C12  *C13 FB      2.4356     32.07     53.03  111.88   1.3452
IC   O    C12  *C13 FC      2.4356     32.07    172.94  109.70   1.3553
!   -------------------   ------- --------- --------- -------  -------
```

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! ***************************************************************************
! 11) -(OCH2CH2)3OH RESIDUE                                        *
!                                                                  *
! Note:  The internal coordinates for the OEG end cap are for a helical       *
! conformation.  The illustration shows a trans conformation for simplicity.  *
! Though the trans conformation is energetically favored in vacuum, the       *
! helical endcap structure is favored when the SAM is solvated in TIP3.       *
!                                                                  *
! SAM MODEL                          PARENT CGenFF RESIdue       *
! ************************           *********************************
RESIdue    PEGH     0.00 !                !
GROUp                 !         HO        ! Hydroxyl charge group from
 ATOM OH   OPEG    -0.65 !        /          ! ETAM (ethanolamine -OH endcap)
 ATOM HO   HGP1     0.42 !      OH           !
 ATOM C17  CG321    0.05 !       |           !
 ATOM H17A HGA2     0.09 !  H17A-C17-H17B      !
 ATOM H17B HGA2     0.09 !       |           !
GROUp                 !                     !
 ATOM C16  CG321   -0.01 !       |           ! Polyethylene glycol monomer
 ATOM H16A HGA2     0.09 !  H16A-C16-H16B      ! charge group from PEGM
 ATOM H16B HGA2     0.09 !       |           !
 ATOM O3   OG301   -0.34 !      O3           !
 ATOM C15  CG321   -0.01 !       |           !
 ATOM H15A HGA2     0.09 !  H15A-C15-H15B      !
 ATOM H15B HGA2     0.09 !       |           !
GROUp                 !                     !
 ATOM C14  CG321   -0.01 !       |           !
 ATOM H14A HGA2     0.09 !  H14A-C14-H14B      !
 ATOM H14B HGA2     0.09 !       |           !
 ATOM O2   OG301   -0.34 !      O2           !
 ATOM C13  CG321   -0.01 !       |           !
 ATOM H13A HGA2     0.09 !  H13A-C13-H13B      !
 ATOM H13B HGA2     0.09 !       |           !
GROUp                 !                     !
 ATOM C12  CG321   -0.01 !       |           !
 ATOM H12A HGA2     0.09 !  H12A-C12-H12B      !
 ATOM H12B HGA2     0.09 !       |           !
 ATOM O1   OG301   -0.34 !      O1           !
 ATOM C11  CG321   -0.01 !       |           !
 ATOM H11A HGA2     0.09 !  H11A-C11-H11B      !
 ATOM H11B HGA2     0.09 !       |           !
GROUp                 !                     !
 ATOM  C10  CG321  -0.18 !  H10A-C10          ! Methylene from HEXA (hexane)
 ATOM  H10A HGA2    0.09 !      / \           !
 ATOM  H10B HGA2    0.09 !    H10B  \         !
GROUp                 !                     !
 ATOM  C09  CG321  -0.18 !         C09-H09A   !
 ATOM  H09A HGA2    0.09 !         / \        !
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 ATOM  H09B HGA2    0.09 !        /  H09B    !
GROUp               !                !
 ATOM  C08  CG321  -0.18 !  H08A-C08         !
 ATOM  H08A HGA2    0.09 !      / \          !
 ATOM  H08B HGA2    0.09 !    H08B  \        !
GROUp               !                !
 ATOM  C07  CG321  -0.18 !         C07-H07A   !
 ATOM  H07A HGA2    0.09 !         / \       !
 ATOM  H07B HGA2    0.09 !        /  H07B    !
GROUp               !                !
 ATOM  C06  CG321  -0.18 !  H06A-C06         !
 ATOM  H06A HGA2    0.09 !      / \          !
 ATOM  H06B HGA2    0.09 !    H06B  \        !
GROUp               !                !
 ATOM  C05  CG321  -0.18 !         C05-H05A   !
 ATOM  H05A HGA2    0.09 !         / \       !
 ATOM  H05B HGA2    0.09 !        /  H05B    !
GROUp               !                !
 ATOM  C04  CG321  -0.18 !  H04A-C04         !
 ATOM  H04A HGA2    0.09 !      / \          !
 ATOM  H04B HGA2    0.09 !    H04B  \        !
GROUp               !                !
 ATOM  C03  CG321  -0.18 !         C03-H03A   !
 ATOM  H03A HGA2    0.09 !         / \       !
 ATOM  H03B HGA2    0.09 !        /  H03B    !
GROUp               !                !
 ATOM  C02  CG321  -0.18 !  H02A-C02         !
 ATOM  H02A HGA2    0.09 !      / \          !
 ATOM  H02B HGA2    0.09 !    H02B  \        !
GROUp               !                !
 ATOM  C01  CG321  -0.11 !         C01-H01A   ! Thiol from CYS (amino acid)
 ATOM  H01A HGA2    0.09 !         / \       !
 ATOM  H01B HGA2    0.09 !        /   H01B   !
                !       /          !
 ATOM  SH   SG311  -0.23 !      SH           !
 ATOM  HS   HGP3    0.16 !       \           !
                !        HS         !
! ************************                  *********************************
BOND     HS  SH
BOND     SH  C01
BOND     C01 C02   C01 H01A  C01 H01B
BOND     C02 C03   C02 H02A  C02 H02B
BOND     C03 C04   C03 H03A  C03 H03B
BOND     C04 C05   C04 H04A  C04 H04B
BOND     C05 C06   C05 H05A  C05 H05B
BOND     C06 C07   C06 H06A  C06 H06B
BOND     C07 C08   C07 H07A  C07 H07B
BOND     C08 C09   C08 H08A  C08 H08B
BOND     C09 C10   C09 H09A  C09 H09B
BOND     C10 C11   C10 H10A  C10 H10B
BOND     C11 O1    C11 H11A  C11 H11B
BOND     O1  C12
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BOND     C12 C13   C12 H12A  C12 H12B
BOND     C13 O2    C13 H13A  C13 H13B
BOND     O2  C14
BOND     C14 C15   C14 H14A  C14 H14B
BOND     C15 O3    C15 H15A  C15 H15B
BOND     O3  C16
BOND     C16 C17   C16 H16A  C16 H16B
BOND     C17 OH    C17 H17A  C17 H17B
BOND     OH  HO

!   i   j   k   l     R(ij/k) T(ijk/kj) PHI(ijkl)  T(jkl)    R(kl)
!   ------------------   ------- --------- --------- -------  -------
IC   C02  C01  SH   HS     1.5239    109.37    179.88   96.90   1.3421
IC   SH   C02  *C01 H01A    1.8249    109.37    120.45  109.88   1.0938
IC   SH   C02  *C01 H01B    1.8249    109.37   -120.40  109.82   1.0940
IC   SH   C01  C02  C03     1.8249    109.37    179.99  112.13   1.5272
IC   C01  C03  *C02 H02A    1.5239    112.13   -121.56  109.53   1.0967
IC   C01  C03  *C02 H02B    1.5239    112.13    121.65  109.54   1.0965
IC   C01  C02  C03  C04     1.5239    112.13   -179.96  112.81   1.5282
IC   C02  C04  *C03 H03A    1.5272    112.81    122.01  109.29   1.0982
IC   C02  C04  *C03 H03B    1.5272    112.81   -121.87  109.20   1.0988
IC   C02  C03  C04  C05     1.5272    112.81   -179.99  113.10   1.5273
IC   C03  C05  *C04 H04A    1.5282    113.10   -121.91  109.34   1.0988
IC   C03  C05  *C04 H04B    1.5282    113.10    122.03  109.37   1.0975
IC   C03  C04  C05  C06     1.5282    113.10   -179.97  113.14   1.5273
IC   C04  C06  *C05 H05A    1.5273    113.14    122.01  109.33   1.0983
IC   C04  C06  *C05 H05B    1.5273    113.14   -121.99  109.28   1.0987
IC   C04  C05  C06  C07     1.5273    113.14    179.99  113.17   1.5267
IC   C05  C07  *C06 H06A    1.5273    113.17   -121.98  109.32   1.0989
IC   C05  C07  *C06 H06B    1.5273    113.17    122.02  109.33   1.0981
IC   C05  C06  C07  C08     1.5273    113.17   -179.91  113.15   1.5272
IC   C06  C08  *C07 H07A    1.5267    113.15    122.04  109.27   1.0992
IC   C06  C08  *C07 H07B    1.5267    113.15   -122.06  109.26   1.0985
IC   C06  C07  C08  C09     1.5267    113.15   -179.91  113.15   1.5273
IC   C07  C09  *C08 H08A    1.5272    113.15   -122.07  109.21   1.0984
IC   C07  C09  *C08 H08B    1.5272    113.15    122.00  109.24   1.0984
IC   C07  C08  C09  C10     1.5272    113.15   -179.97  113.03   1.5279
IC   C08  C10  *C09 H09A    1.5273    113.03    121.95  109.38   1.0984
IC   C08  C10  *C09 H09B    1.5273    113.03   -121.98  109.44   1.0988
IC   C08  C09  C10  C11     1.5273    113.03    179.41  111.72   1.5239
IC   C09  C11  *C10 H10A    1.5279    111.72   -121.69  108.49   1.0960
IC   C09  C11  *C10 H10B    1.5279    111.72    121.41  110.39   1.0971
IC   C09  C10  C11  O1      1.5279    111.72    172.61  113.93   1.4292
IC   C10  O1  *C11  H11A    1.5239    113.93    119.25  104.11   1.0951
IC   C10  O1  *C11  H11B    1.5239    113.93   -125.74  110.35   1.0968
IC   C10  C11  O1   C12     1.5239    113.93     65.43  115.15   1.4205
IC   C11  O1   C12  C13     1.4292    115.15     54.45  114.34   1.5259
IC   O1   C13  *C12 H12A    1.4205    114.34    125.71  108.32   1.1013
IC   O1   C13  *C12 H12B    1.4205    114.34   -117.38  110.78   1.0935
IC   O1   C12  C13  O2      1.4205    114.34     41.02  113.81   1.4233
IC   C12  O2   *C13 H13A    1.5259    113.81   -123.91  111.18   1.0989
IC   C12  O2   *C13 H13B    1.5259    113.81    120.67  104.21   1.0940
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IC   C12  C13  O2   C14    1.5259   113.81    56.79  114.93   1.4223
IC   C13  O2   C14  C15    1.4233   114.93    57.32  113.69   1.5268
IC   O2   C15  *C14 H14A   1.4223   113.69   -116.81  110.82   1.0935
IC   O2   C15  *C14 H14B   1.4223   113.69    124.99  109.42   1.0996
IC   O2   C14  C15  O3     1.4223   113.69    40.18  114.07   1.4197
IC   C14  O3   *C15 H15A   1.5268   114.07    120.91  104.14   1.0934
IC   C14  O3   *C15 H15B   1.5268   114.07   -124.18  111.59   1.1005
IC   C14  C15  O3   C16    1.5268   114.07    56.35  115.32   1.4221
IC   C15  O3   C16  C17    1.4197   115.32    58.07  114.52   1.5157
IC   O3   C17  *C16 H16A   1.4221   114.52    125.35  109.56   1.0991
IC   O3   C17  *C16 H16B   1.4221   114.52   -116.27  108.73   1.0935
IC   O3   C16  C17  OH     1.4221   114.52    54.51  107.87   1.4232
IC   C16  OH   *C17 H17A   1.5157   107.87   -118.33  111.99   1.1008
IC   C16  OH   *C17 H17B   1.5157   107.87    121.76  111.16   1.0999
IC   C16  C17  OH   HO     1.5157   107.87    178.28  107.55   0.9722
!    ------------------   ------- --------- --------- -------  -------

PATChing FIRS NONE LAST NONE

END
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