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*>>>>>>>>> CHARMM22 Proteins and CHARMM27 Lipids <<<<<<<<<<
*from
*>>>> CHARMM22 All-Hydrogen Parameter File for Proteins <<<<<<<<<<
*>>>>>>>>>>>>>>>>>>>> August 1999 <<<<<<<<<<<<<<<<<<<<<<<<<<<<<
*>>>>>>> Direct comments to Alexander D. MacKerell Jr. <<<<<<<<<
*>>>>>> 410-706-7442 or email: alex,mmiris.ab.umd.edu  <<<<<<<<<
*and
*\\\\\\\ CHARMM27 All-Hydrogen Lipid Parameter File ///////
*\\\\\\\\\\\\\\\\\\ Developmental ////////////////////////

*  ------------------------------------------------------------------------  *
*         CGenFF: Parameters for the Charmm General Force Field v. 2b8       *
*                    for Small Molecule Drug Design                          *
*  ------------------------------------------------------------------------  *
!  ------------------------------------------------------------------------  !
!  Reference: K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong,  !
!      J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov and             !
!      A. D. Mackerell Jr., J. Comput. Chem. 2010, 31, 671-690.              !
!  ------------------------------------------------------------------------  !
!  Notes: - CGenFF is an ongoing project that is updated regularly. Please   !
!             check http://dogmans.umaryland.edu/~kenno/cgenff/download.html !
!             and/or http://mackerell.umaryland.edu/ for updates!            !
!         - As more functional groups will be introduced, small changes in   !
!             existing parameters and/or charges may occur.                  !
!         - Comments in this file may be misleading.                         !
!  ------------------------------------------------------------------------  !
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!                xhe   = Xibing He                                           !
!                xxwy  = Wenbo Yu                                            !
!                yapol = Iakov Polyak                                        !
!                yin   = Daxu Yin                                            !
!  ------------------------------------------------------------------------  !
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!  All comments to ADM jr. via the CHARMM web site: www.charmm.org             !
!                parameter set discussion forum                               !
!  ------------------------------------------------------------------------   !
!  ORDER OF PREFERENCE FOR SORTING PARAMETERS:                                 !
!         + C < N < O < P < S < HALOGENS (LOW TO HIGH Z) < MISC. (BY Z) < H    !
!         + ATOMS TYPES WITHIN THE SAME ELEMENT ARE SORTED ALPHABETICALLY      !
!  ------------------------------------------------------------------------   !
!  RULES FOR SORTING THE COLUMS ON EACH LINE:                                  !
!         + IN BONDS, THE LOWEST PRIORITY ATOM ALWAYS COMES FIRST              !
!         + FOR ANGLES, IF COLUMN 3 HAS A LOWER PRIORITY THAN COLUMN 1,        !
!           COLUMNS 1 & 3 ARE SWAPPED                                          !
!         + FOR DIHEDRALS, IF COLUMN 3 HAS LOWER PRIORITY THAN COLUMN 2, THE   !
!           ORDER FOR THE ENTIRE DIHEDRAL IS REVERSED                          !
!         + FOR DIHEDRALS, IF COLUMNS 2 & 3 HAVE THE SAME PRIORITY, COLUMS     !
!           1 & 4 ARE CONSIDERED INSTEAD. IF 4 HAS LOWER PRIORITY THAN 1, THE  !
!           ORDER FOR THE ENTIRE DIHEDRAL IS REVERSED                          !
!         + FOR IMPROPERS, NO SORTING IS PERFORMED *AFTER* PARAMETRIZATION,    !
!           BUT THE FOLLOWING RULES APPLY *DURING* PARAMETRIZATION:            !
!               - COLUMN 1 IS ALWAYS THE CENTRAL ATOM                          !
!               - IF 2 OF THE SUBSTITUENTS HAVE IDENTICAL TYPES, THESE SHOULD  !
!                 BE IN COLUMNS 2 & 3 (BUT THEY CANNOT BE MOVED AROUND         !
!                 WITHOUT RE-OPTIMIZING THE PARAMETER)                         !
!               - IF THE SUBSTITUENTS ARE ALL DIFFERENT, COLUMNS 2, 3 & 4      !
!                 SHOULD BE SORTED BY INCREASING PRIORITY. COLUMNS 2 AND 3     !
!                 CAN BE SWAPPED WITHOUT CHANGING THE PARAMETER BUT OTHER      !
!                 PERMUTATIONS MANDATE RE-OPTIMIZATION                         !
!  ------------------------------------------------------------------------   !
!  PRIORITY OF COLUMNS FOR THE PURPOSE OF SORTING THE LINES IN EACH SECTION:   !
!          BONDS     -- 1,2                                                    !
!          ANGLES    -- 2,1,3                                                  !
!          DIHEDRALS -- 2,3,1,4                                                !
!          IMPROPERS -- 1,4,2,3                                                !
!  WHERE 1,2,3,4 INDICATE COLUMN NO, EG. ANGLES ARE FIRST SORTED BY COLUMN 2,  !
!  THEN (IF COLUMN 2 IS THE SAME) BY COLUMN 1, THEN BY COLUMN 3.               !
!  ------------------------------------------------------------------------   !



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BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom types  Kb         b0
!
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!!  CENTRAL RING (revision 6/2014)
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!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CG2R61A   CG2R61B    305.000     1.397
CG2R61A   CG2R61C    305.000     1.397
CG2R61A   CG2R61D    305.000     1.397
        ! Kb = PROT benzene, JES 8/25/89
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
        ! b0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
        ! Results used are averages of both molecules, differ < 1%
HGR61   CG2R61B    340.000     1.081
HGR61   CG2R61C    340.000     1.081
HGR61   CG2R61D    340.000     1.081
        ! Kb = PROT phe,tyr JES 8/25/89
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
        ! b0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
        ! Results used are averages of both molecules, differ < 1%
CG2DC1A  CG2R61A     365.000     1.4635
CG2DC1B  CG2R61A     365.000     1.4635
CG2DC1C  CG2R61A     365.000     1.4635
        ! Kb = compromise between HDZ1B and STYR by kevo
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
CG2DC1A  CG2DC1D   440.000     1.3500
CG2DC1B  CG2DC1D   440.000     1.3500
CG2DC1C  CG2DC1D   440.000     1.3500
        ! Kb = RETINOL BTE2, 2-butene
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
HGA4  CG2DC1A   360.500     1.0853
HGA4  CG2DC1B   360.500     1.0853
HGA4  CG2DC1C   360.500     1.0853
        ! Kb = LIPID propene, yin/adm jr., 12/95
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014


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!!  PERIPHERAL RING (revision 6/2014)  *** Note Repeated entries ***
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CG2R61A   CG2R61B    305.000     1.397
!CG2R61A   CG2R61C    305.000     1.397
!CG2R61A   CG2R61D    305.000     1.397
CG2R61B   CG2R61B    305.000     1.397
CG2R61C   CG2R61C    305.000     1.397
CG2R61B   CG2R61D    305.000     1.397
CG2R61C   CG2R61D    305.000     1.397
          ! Kb = PROT benzene, JES 8/25/89
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
        ! b0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
        ! Results used are averages of both molecules, differ < 1%
!HGR61   CG2R61B    340.000     1.081
!HGR61   CG2R61C    340.000     1.081
!HGR61   CG2R61D    340.000     1.081
          ! Kb = PROT phe,tyr JES 8/25/89
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
        ! b0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
        ! Results used are averages of both molecules, differ < 1%
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```
HGA4  CG2DC1D   360.500     1.0853
        ! Kb = LIPID propene, yin/adm jr., 12/95
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
CG2DC1D  CG2R61A     365.000     1.463545
        ! Kb = compromise between HDZ1B and STYR by kevo
        ! b0 = MP2/631gdp stilbene, A. St. John, 5/2014
OG301   CG2R61B    230.00     1.3728
OG301   CG2R61C    230.00     1.3728
        ! Kb = COMPDS peml
        ! b0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014


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!!  Oxygen + Alkane branches
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OG301   CG321    360.000     1.4252
        ! Kb = diethylether, alex (not our alex)
        ! b0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
CG321  CG321   222.500     1.5243
           ! Kb = alkane update, adm jr., 3/2/92
        ! b0 = MP2/631gdp Hexane, A. St. John, 5/2014
        ! (1,3-diethoxy-5-methylbenzene differs by ~ 1%, bond nearest to oxygen)
CG331  CG321   222.500     1.5236
           ! Kb =  alkane update, adm jr., 3/2/92
        ! b0 = MP2/631gdp Hexane, A. St. John, 5/2014
HGA2   CG321   309.000     1.093
           ! Kb = alkane update, adm jr., 3/2/92
        ! b0 = MP2/631gdp Hexane, A. St. John, 5/2014
HGA3   CG331   322.000     1.089
           ! Kb = alkane update, adm jr., 3/2/92
        ! b0 = MP2/631gdp Hexane, A. St. John, 5/2014

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!!  Graphite
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CG2R61   CG2R61    305.000     1.397




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ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
!
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!!  CENTRAL RING (revision 6/2014)
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CG2R61A   CG2R61B   CG2R61A    40.000    120.00   35.00   2.41967
CG2R61A   CG2R61C   CG2R61A    40.000    120.00   35.00   2.41967
CG2R61A   CG2R61D   CG2R61A    40.000    120.00   35.00   2.41967
CG2R61B   CG2R61A   CG2R61C    40.000    120.00   35.00   2.41967
CG2R61C   CG2R61A   CG2R61D    40.000    120.00   35.00   2.41967
CG2R61D   CG2R61A   CG2R61B    40.000    120.00   35.00   2.41967
        ! Ktheta = PROT JES 8/25/89
        ! S0 correct from JES and from ASJ (2014)
HGR61   CG2R61B   CG2R61A    30.000    120.00   22.00   2.15265
HGR61   CG2R61C   CG2R61A    30.000    120.00   22.00   2.15265
HGR61   CG2R61D   CG2R61A    30.000    120.00   22.00   2.15265
        ! Ktheta = JES 8/25/89
        ! S0 correct from JES and from ASJ (2014)
CG2R61D  CG2R61A    CG2DC1A   36.00    122.41
CG2R61B  CG2R61A    CG2DC1A   36.00    117.23
CG2R61B  CG2R61A    CG2DC1C   36.00    122.41
CG2R61C  CG2R61A    CG2DC1C   36.00    117.23
CG2R61C  CG2R61A    CG2DC1B   36.00    122.41
CG2R61D  CG2R61A    CG2DC1B   36.00    117.23
        ! Ktheta = STYR, styrene & HDZ2, hydrazone model cmpd 2; xxwy & oashi; verified by kevo
        ! Theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
HGA4  CG2DC1A  CG2DC1D    42.00    118.876
HGA4  CG2DC1B  CG2DC1D    42.00    118.876
HGA4  CG2DC1C  CG2DC1D    42.00    118.876
HGA4  CG2DC1D  CG2DC1A    42.00    118.876
HGA4  CG2DC1D  CG2DC1B    42.00    118.876
HGA4  CG2DC1D  CG2DC1C    42.00    118.876
        ! Ktheta = RETINOL BTE2, 2-butene
        ! Theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
CG2R61A  CG2DC1A   CG2DC1D   48.00    125.199
CG2R61A  CG2DC1B   CG2DC1D   48.00    125.199
CG2R61A  CG2DC1C   CG2DC1D   48.00    125.199
        ! *********Ktheta=48.00 GUESS by Michael Roth -- WE WILL ACCEPT BUTENE (not
        styrene)**********
        ! Ktheta = CG2D1  CG2D1  CG321    48.00    123.50 ! LIPID  2-butene, yin,adm jr., 12/95
        !         CG2DC3 CG2DC1 CG2R61   29.00    122.00 ! STYR, styrene, xxwy & oashi
        ! Theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
CG2R61A   CG2DC1A  HGA4   32.00    115.910
CG2R61A   CG2DC1B  HGA4   32.00    115.910
CG2R61A   CG2DC1C  HGA4   32.00    115.910
CG2R61A   CG2DC1D  HGA4   32.00    115.910
        !  ******** WE WILL GO WITH THE conjugated version (hydrazone model, styrene)
        ! Ktheta = HDZ1b, hydrazone model cmpd 1b; STYR, styrene; kevo, xxwy, oashi
        !   (non-conjugated) CG2D1  CG2D1  HGA4     52.00    119.50 ! LIPID 2-butene, yin,adm
        jr., 12/95
        ! Theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
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!!  PERIPHERAL RING (revision 6/2014)  *** Note Repeated entries ***
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CG2R61A   CG2R61B   CG2R61B    40.000    120.00   35.00   2.41967
CG2R61B   CG2R61B   CG2R61D    40.000    120.00   35.00   2.41967
CG2R61B   CG2R61D   CG2R61C    40.000    120.00   35.00   2.41967
CG2R61D   CG2R61C   CG2R61C    40.000    120.00   35.00   2.41967
CG2R61C   CG2R61C   CG2R61A    40.000    120.00   35.00   2.41967
!CG2R61C   CG2R61A   CG2R61B    40.000    120.00   35.00   2.41967
        ! Ktheta = PROT JES 8/25/89 benzene
        ! S0 correct from JES and from ASJ (2014)
!HGR61   CG2R61B   CG2R61A    30.000    120.00   22.00   2.15265
!HGR61   CG2R61C   CG2R61A    30.000    120.00   22.00   2.15265
HGR61   CG2R61C   CG2R61C    30.000    120.00   22.00   2.15265
HGR61   CG2R61B   CG2R61B    30.000    120.00   22.00   2.15265
HGR61   CG2R61D   CG2R61B    30.000    120.00   22.00   2.15265
HGR61   CG2R61D   CG2R61C    30.000    120.00   22.00   2.15265
        ! Ktheta = PROT JES 8/25/89 benzene
        ! S0 correct from JES and from ASJ (2014)
OG301   CG2R61C   CG2R61C    110.00   124.22
OG301   CG2R61C   CG2R61D    110.00   117.77
OG301   CG2R61B   CG2R61D    110.00   124.22
OG301   CG2R61B   CG2R61B    110.00   117.77
        ! Ktheta = BIPHENYL ANALOGS, peml
        ! Theta0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
CG2R61B   OG301   CG321    65.00   117.43
CG2R61C   OG301   CG321    65.00   117.43
        ! Ktheta = ETOB, Ethoxybenzene, cacha, MEOB, Methoxybenzene, cacha
        ! Theta0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
CG2R61A  CG2DC1D   CG2DC1A   48.00    125.199
CG2R61A  CG2DC1D   CG2DC1B   48.00    125.199
CG2R61A  CG2DC1D   CG2DC1C   48.00    125.199
        ! *********Ktheta=48.00 GUESS by Michael Roth -- WE WILL ACCEPT BUTENE (not
        styrene)**********
        ! Ktheta = CG2D1  CG2D1  CG321    48.00    123.50 ! LIPID  2-butene, yin,adm jr., 12/95
        !         CG2DC3 CG2DC1 CG2R61   29.00    122.00 ! STYR, styrene, xxwy & oashi
        ! Theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
!CG2R61A   CG2DC1D  HGA4   32.00    115.910
        !  ******** WE WILL GO WITH THE conjugated version (hydrazone model, styrene)
        !   (non-conjugated) CG2D1  CG2D1  HGA4     52.00    119.50 ! LIPID 2-butene, yin,adm
        jr., 12/95
        ! Ktheta = HDZ1b, hydrazone model cmpd 1b; STYR, styrene; kevo, xxwy, oashi
        ! Theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
CG2R61B  CG2R61A    CG2DC1D   36.00    124.22
        ! Ktheta = STYR, styrene & HDZ2, hydrazone model cmpd 2; xxwy & oashi; verified by kevo
        ! theta0 = MP2/631gdp stilbene, A. St. John, 5/2014
CG2R61C  CG2R61A    CG2DC1D   36.00    117.77
        ! Ktheta = STYR, styrene & HDZ2, hydrazone model cmpd 2; xxwy & oashi; verified by kevo
        ! theta0 = MP2/631gdp stilbene, A. St. John, 5/2014

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!!  Oxygen + Alkane branches
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CG321 CG321 OG301      45.000    106.805
        ! Ktheta = diethylether, alex (not our alex)
        ! Theta0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
        ! We are removing the UB term (Mike's) since the cgenff file does not have it
OG301   CG321  HGA2     45.900   110.013
        ! Ktheta = ETOB, Ethoxybenzene, cacha
        ! Theta0 = MP2/631gdp 1,3-diethoxy-5-methylbenzene, A. St. John, 5/2014
CG321  CG321  CG321   58.350    113.4205   11.16   2.54834
        ! Ktheta = alkane update, adm jr., 3/2/92
        ! Theta0 = MP2/631gdp hexane, A. St. John (5/2014)
        ! first angle (next to O) is 112.9 (difference neglected)
        ! S0 correct from alkane ASJ (2014) geometry
CG331  CG321  CG321   58.000    112.904    8.00   2.54776
        ! Ktheta = alkane update, adm jr., 3/2/92
        ! Theta0 = MP2/631gdp hexane, A. St. John (5/2014)
        ! S0 correct from alkane ASJ (2014) geometry
HGA2   CG321  CG321   26.500    109.350   22.53   2.14993
HGA2   CG321  CG331   34.600    109.612   22.53   2.15265
HGA3   CG331  CG321   34.600    111.025   22.53   2.16745
HGA3   CG331  HGA3    35.500    107.770    5.40   1.74399
        ! Ktheta = alkane update, adm jr., 3/2/92
        ! Theta0 = MP2/631gdp hexane, A. St. John (5/2014)
        ! S0 from geometry (ASJ 7-2014)
HGA2   CG321  HGA2    35.500    106.400    5.40   1.76593
        ! Ktheta = alkane update, adm jr., 3/2/92
        ! Theta0 = MP2/631gdp hexane, A. St. John (5/2014)
        ! one closest to O is ~ 1.5 deg. bigger
        ! S0 from geometry (ASJ 7-2014)

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!!  Graphite
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CG2R61   CG2R61   CG2R61    40.000    120.00   35.00   2.41967



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DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!
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!!  CENTRAL RING (revision 6/2014)
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CG2R61A   CG2R61B   CG2R61A   CG2R61D       3.1000  2   180.00
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CG2R61B   CG2R61A   CG2R61D   CG2R61A       3.1000  2   180.00
CG2R61A   CG2R61D   CG2R61A   CG2R61C       3.1000  2   180.00
CG2R61D   CG2R61A   CG2R61C   CG2R61A       3.1000  2   180.00
CG2R61A   CG2R61C   CG2R61A   CG2R61B       3.1000  2   180.00
CG2R61C   CG2R61A   CG2R61B   CG2R61A       3.1000  2   180.00
            ! Kchi = PROT JES 8/25/89 benzene
HGR61   CG2R61B   CG2R61A   CG2R61D       4.2000  2   180.00
HGR61   CG2R61B   CG2R61A   CG2R61C       4.2000  2   180.00
HGR61   CG2R61D   CG2R61A   CG2R61B       4.2000  2   180.00
HGR61   CG2R61D   CG2R61A   CG2R61C       4.2000  2   180.00
HGR61   CG2R61C   CG2R61A   CG2R61D       4.2000  2   180.00
HGR61   CG2R61C   CG2R61A   CG2R61B       4.2000  2   180.00
            ! Kchi = PROT JES 8/25/89 benzene
HGR61 CG2R61B CG2R61A CG2DC1A   2.4000  2   180.00
HGR61 CG2R61B CG2R61A CG2DC1C   2.4000  2   180.00
HGR61 CG2R61D CG2R61A CG2DC1A   2.4000  2   180.00
HGR61 CG2R61D CG2R61A CG2DC1B   2.4000  2   180.00
HGR61 CG2R61C CG2R61A CG2DC1B   2.4000  2   180.00
HGR61 CG2R61C CG2R61A CG2DC1C   2.4000  2   180.00
            ! Kchi = HDZ2, hydrazone model cmpd 2 Kenno: 4.2 -> 2.4
CG2R61A CG2R61B CG2R61A CG2DC1A  3.1000  2   180.00
CG2R61A CG2R61C CG2R61A CG2DC1B  3.1000  2   180.00
CG2R61A CG2R61B CG2R61A CG2DC1C  3.1000  2   180.00
CG2R61A CG2R61D CG2R61A CG2DC1B  3.1000  2   180.00
CG2R61A CG2R61D CG2R61A CG2DC1A  3.1000  2   180.00
CG2R61A CG2R61C CG2R61A CG2DC1C  3.1000  2   180.00
            ! Kchi = HDZ2, hydrazone model cmpd 2
CG2R61D CG2R61A CG2DC1A CG2DC1D   0.7500  2   180.00
CG2R61D CG2R61A CG2DC1A CG2DC1D   0.1900  4     0.00
CG2R61B CG2R61A CG2DC1A CG2DC1D   0.7500  2   180.00
CG2R61B CG2R61A CG2DC1A CG2DC1D   0.1900  4     0.00
CG2R61B CG2R61A CG2DC1C CG2DC1D   0.7500  2   180.00
CG2R61B CG2R61A CG2DC1C CG2DC1D   0.1900  4     0.00
CG2R61C CG2R61A CG2DC1C CG2DC1D   0.7500  2   180.00
CG2R61C CG2R61A CG2DC1C CG2DC1D   0.1900  4     0.00
CG2R61C CG2R61A CG2DC1B CG2DC1D   0.7500  2   180.00
CG2R61C CG2R61A CG2DC1B CG2DC1D   0.1900  4     0.00
CG2R61D CG2R61A CG2DC1B CG2DC1D   0.7500  2   180.00
CG2R61D CG2R61A CG2DC1B CG2DC1D   0.1900  4     0.00
            ! ***************APPROX**************
            ! Kchi = STYR, styrene, xxwy & oashi
            !
            ! with these parameters we get "shallow basin" at 0 and 180 degrees
            ! actual minimum at around 4.6 degrees, delta E = 0.38 kcal/mol
CG2R61B CG2R61A CG2DC1A HGA4   0.6000  2     180.00
CG2R61B CG2R61A CG2DC1C HGA4   0.6000  2     180.00
CG2R61C CG2R61A CG2DC1B HGA4   0.6000  2     180.00
CG2R61C CG2R61A CG2DC1C HGA4   0.6000  2     180.00
CG2R61D CG2R61A CG2DC1A HGA4   0.6000  2     180.00
CG2R61D CG2R61A CG2DC1B HGA4   0.6000  2     180.00
            ! Kchi = HDZ1b, hydrazone model cmpd 1b, kevo
X   CG2DC1A  CG2DC1D  X        5.2000  2   180.00
X   CG2DC1B  CG2DC1D  X        5.2000  2   180.00
```

```
X   CG2DC1C  CG2DC1D  X        5.2000  2   180.00
            ! Kchi = butene, yin/adm jr., 12/95
            !
            ! ***********WILDCARDS************
            ! CG2R61A CG2DC1A CG2DC1D HGA4
            ! CG2R61A CG2DC1B CG2DC1D HGA4
            ! CG2R61A CG2DC1C CG2DC1D HGA4
            ! HGA4 CG2DC1A CG2DC1D HGA4
            ! HGA4 CG2DC1B CG2DC1D HGA4
            ! HGA4 CG2DC1C CG2DC1D HGA4
            ! CG2R61A CG2DC1A CG2DC1D CG2R61A
            ! CG2R61A CG2DC1B CG2DC1D CG2R61A
            ! CG2R61A CG2DC1C CG2DC1D CG2R61A
            ! ********************************
            !
            ! the barrier between trans and cis is VERY HIGH (> 6,000 K)
            ! hence, trans <-> cis transitions NEVER happen
            ! Kchi=5.2 maintains the INITIAL (trans) CONFIGURATION (either 0 or 180 deg.)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!  PERIPHERAL RING (revision 6/2014) (Note repeated entries)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CG2R61B CG2R61A CG2DC1D CG2DC1A   0.7500  2   180.00
CG2R61B CG2R61A CG2DC1D CG2DC1A   0.1900  4     0.00
CG2R61B CG2R61A CG2DC1D CG2DC1B   0.7500  2   180.00
CG2R61B CG2R61A CG2DC1D CG2DC1B   0.1900  4     0.00
CG2R61B CG2R61A CG2DC1D CG2DC1C   0.7500  2   180.00
CG2R61B CG2R61A CG2DC1D CG2DC1C   0.1900  4     0.00
CG2R61C CG2R61A CG2DC1D CG2DC1A   0.7500  2   180.00
CG2R61C CG2R61A CG2DC1D CG2DC1A   0.1900  4     0.00
CG2R61C CG2R61A CG2DC1D CG2DC1B   0.7500  2   180.00
CG2R61C CG2R61A CG2DC1D CG2DC1B   0.1900  4     0.00
CG2R61C CG2R61A CG2DC1D CG2DC1C   0.7500  2   180.00
CG2R61C CG2R61A CG2DC1D CG2DC1C   0.1900  4     0.00
            ! *************APPROX**************
            ! Kchi = STYR, styrene, xxwy & oashi
            !
            ! with these parameters we get "shallow basin" at 0 and 180 degrees
            ! actual minimum at around 4.6 degrees, delta E = 0.38 kcal/mol
X    CG2DC1D  CG2DC1A  X        5.2000  2   180.00
X    CG2DC1D  CG2DC1B  X        5.2000  2   180.00
X    CG2DC1D  CG2DC1C  X        5.2000  2   180.00
            ! Kchi = butene, yin/adm jr., 12/95
            !
            !***********WILDCARDS**********
            ! CG2R61A CG2DC1D CG2DC1A HGA4
            ! CG2R61A CG2DC1D CG2DC1B HGA4
            ! CG2R61A CG2DC1D CG2DC1C HGA4
            !*******************************
            !
            ! the barrier between trans and cis is VERY HIGH (> 6,000 K)
            ! hence, trans <-> cis transitions NEVER happen
            ! Kchi=5.2 maintains the INITIAL (trans) CONFIGURATION (either 0 or 180 deg.)
```

```
CG2R61B CG2R61A CG2DC1D HGA4   0.6000  2     180.00
CG2R61C CG2R61A CG2DC1D HGA4   0.6000  2     180.00
            ! Kchi = HDZ1b, hydrazone model cmpd 1b, kevo
CG2R61B CG2R61B CG2R61A CG2DC1D  3.1000  2   180.00
CG2R61C CG2R61C CG2R61A CG2DC1D  3.1000  2   180.00
            ! Kchi = HDZ2, hydrazone model cmpd 2
HGR61 CG2R61B CG2R61A CG2DC1D   2.4000  2   180.00
HGR61 CG2R61C CG2R61A CG2DC1D   2.4000  2   180.00
            ! Kchi = HDZ2, hydrazone model cmpd 2 Kenno: 4.2 -> 2.4
CG2R61A   CG2R61B   CG2R61B   CG2R61D       3.1000  2   180.00
CG2R61B   CG2R61B   CG2R61D   CG2R61C       3.1000  2   180.00
CG2R61B   CG2R61D   CG2R61C   CG2R61C       3.1000  2   180.00
CG2R61D   CG2R61C   CG2R61C   CG2R61A       3.1000  2   180.00
CG2R61C   CG2R61C   CG2R61A   CG2R61B       3.1000  2   180.00
CG2R61C   CG2R61A   CG2R61B   CG2R61B       3.1000  2   180.00
            ! Kchi = PROT JES 8/25/89 benzene
HGR61   CG2R61D   CG2R61B   CG2R61B       4.2000  2   180.00
HGR61   CG2R61D   CG2R61C   CG2R61C       4.2000  2   180.00
!HGR61   CG2R61B   CG2R61A   CG2R61C       4.2000  2   180.00
HGR61   CG2R61B   CG2R61B   CG2R61D       4.2000  2   180.00
HGR61   CG2R61C   CG2R61C   CG2R61D       4.2000  2   180.00
!HGR61   CG2R61C   CG2R61A   CG2R61B       4.2000  2   180.00
            ! Kchi = PROT JES 8/25/89 benzene
CG2R61A CG2R61B CG2R61B OG301     3.1000  2   180.00
CG2R61A CG2R61C CG2R61C OG301     3.1000  2   180.00
CG2R61C CG2R61D CG2R61B OG301     3.1000  2   180.00
CG2R61B CG2R61D CG2R61C OG301     3.1000  2   180.00
            ! Kchi = BIPHENYL ANALOGS, peml
HGR61 CG2R61B CG2R61B OG301    2.4000  2   180.00
HGR61 CG2R61D CG2R61B OG301    2.4000  2   180.00
HGR61 CG2R61D CG2R61C OG301    2.4000  2   180.00
HGR61 CG2R61C CG2R61C OG301    2.4000  2   180.00
            ! Kchi = BIPHENYL ANALOGS, peml. Kenno: 4.2 -> 2.4

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!  Oxygen + Alkane branches
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CG2R61B CG2R61B OG301  CG321      1.6200  2   180.00
CG2R61B CG2R61B OG301  CG321      0.1900  4   180.00
CG2R61D CG2R61B OG301  CG321      1.6200  2   180.00
CG2R61D CG2R61B OG301  CG321      0.1900  4   180.00
CG2R61C CG2R61C OG301  CG321      1.6200  2   180.00
CG2R61C CG2R61C OG301  CG321      0.1900  4   180.00
CG2R61D CG2R61C OG301  CG321      1.6200  2   180.00
CG2R61D CG2R61C OG301  CG321      0.1900  4   180.00
            ! Kchi = ETOB, Ethoxybenzene, cacha
CG321  CG321  OG301  CG2R61B     0.2400  1     0.00
CG321  CG321  OG301  CG2R61B     0.2900  2     0.00
CG321  CG321  OG301  CG2R61B     0.0200  3     0.00
CG321  CG321  OG301  CG2R61C     0.2400  1     0.00
CG321  CG321  OG301  CG2R61C     0.2900  2     0.00
CG321  CG321  OG301  CG2R61C     0.0200  3     0.00
            ! PNTM, pentamidine; from ETOB, Ethoxybenzene; kevo
```

```
            !
            ! **************SEE oxygen_dihedrals_questions.nb for plots******************
            !
            !  ********* THIS ALONE IS GIVING A WEAK MINIMUM AT ~95 degrees, STRANGE ***********
            ! However, adding the other relevant dihedrals that are linked (e.g., involving
            H's) adds
            ! 2*U[chi, .095, 3, 0] + 2 U[chi, .19, 3, 0]
            ! this results in minima at 67 degrees, and a slightly more energetic one at 180
            degrees (this should be the one)
HGA2    CG321   OG301   CG2R61B     0.0950  3     0.00
HGA2    CG321   OG301   CG2R61C     0.0950  3     0.00
            ! ETOB, Ethoxybenzene, cacha
            ! this looks good, +- 60 degrees (and a weird one at 180 degrees)
CG321   CG321   CG321   CG321      0.1500  1     0.00
            ! ***UNKNOWN SOURCE***
                ! Kchi = alkane update, adm jr., 3/2/92, butane trans/gauche
            !
            ! adding numerous dihedrals(4*H2-CT2-CT2-H2, 8*H2-CT2-CT2-CT2 WC)
            ! results in minima at (180 deg, 0 K) and (60 deg, 113 K)
            !
            ! **************SEE alkane_dihedrals_CT2CT2CT2CT2.nb/.pdf for
            plots******************
            !
            ! ***LIPIDS SOURCE***
            ! CTL2 CTL2 CTL2 CTL2     0.101   2     0.00 ! alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL2     0.142   3   180.00 ! alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL2     0.074   4     0.00 ! alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL2     0.097   5     0.00 ! alkane, 7/08, jbk
            ! using the lipids file (2,3,4,5 params)
            ! adding the numerous H dihedrals (4*H2-CT2-CT2-H2, 8*H2-CT2-CT2-CT2 WC)
            ! results in minima at (58.6 deg, 0), (180 deg, 62 K)
            ! note this is NOT including any non-bonded interactions and also is NOT optimized.
            ! barrier height is maximum at (121.1 deg, 2232.4 K)
            !
            ! ***CGENFF SOURCE***
            ! CG321  CG321  CG321  CG321      0.06450 2     0.00 ! LIPID alkane, 4/04, jbk
            (Jeff Klauda)
            ! CG321  CG321  CG321  CG321      0.14975 3   180.00 ! LIPID alkane, 4/04, jbk
            ! CG321  CG321  CG321  CG321      0.09458 4     0.00 ! LIPID alkane, 4/04, jbk
            ! CG321  CG321  CG321  CG321      0.11251 5     0.00 ! LIPID alkane, 4/04, jbk
            ! using the cgenff file (2,3,4,5 params)
            ! adding the numerous H dihedrals (4*H2-CT2-CT2-H2, 8*H2-CT2-CT2-CT2 WC)
            ! results in minima at (58 deg, 0), (180 deg, 41.5 K)
            ! note this is NOT including any non-bonded interactions and also is NOT optimized.
            ! barrier height is maximum at (120.9 deg, 2219.3 K)
CG331   CG321   CG321   CG321      0.1500  1     0.00
            ! ***UNKNOWN SOURCE***
            ! Kchi = alkane update, adm jr., 3/2/92, butane trans/gauche
            !
            ! adding numerous dihedrals(4*H2-CT2-CT2-H2, 8*H2-CT2-CT2-CT2 WC)
            ! results in minima at (180 deg, 0 K) and (60 deg, 113 K)
            !
            ! **************SEE alkane_dihedrals_CT3CT2CT2CT2.nb/.pdf for
```

```
            plots*******************
            !
            ! bare CT2-CT2-CT2-CT3 gives minimum at 180 degrees, reasonable, but missing gauche
            defects, and appears too shallow
            ! adding the numerous H dihedrals (4*H2-CT2-CT2-H2, 2*H2-CT2-CT2-CT3 WC,
            2*H2-CT2-CT2-CT2 WC)
            ! results in minima at (180 deg, 0), (60.4 deg, 113 K)
            ! note this is NOT including any non-bonded interactions and also is NOT optimized.
            ! barrier height is maximum at (120 deg, 2175 K)
            !
            ! ***LIPIDS SOURCE***
            ! CTL2 CTL2 CTL2 CTL3     0.162   2     0.00 ! (lipds) alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL3     0.047   3   180.00 ! (lipds) alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL3     0.105   4     0.00 ! (lipds) alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL3     0.177   5     0.00 ! (lipds) alkane, 7/08, jbk
            ! using the lipids file (2,3,4,5 params)
            ! bare CT2-CT2-CT2-CT3 gives min. at (111 deg, 0), (40 deg, 55 K), (180 deg, 231 K)
            ! adding the numerous H dihedrals (4*H2-CT2-CT2-H2, 2*H2-CT2-CT2-CT3 WC,
            2*H2-CT2-CT2-CT2 WC)
            ! results in minima at (57 deg, 0), (180 deg, 78 K)
            ! note this is NOT including any non-bonded interactions and also is NOT optimized.
            ! barrier height is maximum at (122 deg, 2019 K)
            !
            ! ***CGENFF SOURCE***
            ! CTL2 CTL2 CTL2 CTL3     0.15051   2     0.00 ! (lipds) alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL3     0.08133   3   180.00 ! (lipds) alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL3     0.10824   4     0.00 ! (lipds) alkane, 7/08, jbk
            ! CTL2 CTL2 CTL2 CTL3     0.20391   5     0.00 ! (lipds) alkane, 7/08, jbk
            ! using the cgenff file (2,3,4,5 params)
            ! adding the numerous H dihedrals (4*H2-CT2-CT2-H2, 2*H2-CT2-CT2-CT3 WC,
            2*H2-CT2-CT2-CT2 WC)
            ! results in minima at (57 deg, 0), (180 deg, 56 K)
            ! note this is NOT including any non-bonded interactions and also is NOT optimized.
            ! barrier height is maximum at (123 deg, 1977 K)
! CW NOTE:  WHICH SHOULD WE KEEP??? *************************
! ASJ NOTE: WE WANT UNKNOWN SOURCE (adding H dihedrals(4*H2-CT2-CT2-H2, 8*H2-CT2-CT2-CT2 WC)
results in minima at (180 deg, 0 K) and (60 deg, 113 K))

HGA2   CG321  CG321  HGA2       0.2200  3     0.00
            ! Kchi = LIPID alkanes
HGA2   CG321  CG331  HGA3        0.1600  3     0.00
            ! Kchi = PROT rotation barrier in Ethane (SF)
X      CG321  CG321  X        0.1900  3     0.00
            ! Kchi = (lipids) alkane, 4/98, yin and mackerell
            ! HGA2 CG321 CG321 CG321
            ! OG301 CG321 CG321 HGA2
            ! OG301 CG321 CG321 CG321
X      CG321  CG331  X        0.1600  3     0.00
            ! Kchi = (lipids) alkane, 4/98, yin and mackerell
            ! HGA3 CG331 CG321 CG321

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!  Graphite
```

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CG2R61   CG2R61   CG2R61   CG2R61       3.1000  2   180.00



!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
NONBONDED nbxmod  5 atom cdiel fshift vatom vdistance vfswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   eps,1-4       Rmin/2,1-4
!
!see mass list above for better description of atom types


!hydrogens
HGR61    0.0       -0.0300     1.3582 ! benzene
HGA2     0.0       -0.0350     1.3400 ! alkane, igor, 6/05
HGA3     0.0       -0.0240     1.3400 ! alkane, yin and mackerell, 4/98
HGA4     0.0       -0.0310     1.2500 ! alkene, yin,adm jr., 12/95

!carbons
CG321    0.0       -0.0560     2.0100   0.0 -0.01 1.9 ! alkane (CT2), 4/98, yin, adm jr, also
used by viv
CG331    0.0       -0.0780     2.0500   0.0 -0.01 1.9 ! alkane (CT3), 4/98, yin, adm jr; Rmin/2
modified from 2.04 to 2.05
CG2R61   0.0       -0.0700     1.9924 ! INDO/TRP
CG2R61A   0.0       -0.0700     1.9924 ! INDO/TRP
CG2R61B   0.0       -0.0700     1.9924 ! INDO/TRP
CG2R61C   0.0       -0.0700     1.9924 ! INDO/TRP
CG2R61D   0.0       -0.0700     1.9924 ! INDO/TRP
CG2DC1   0.0       -0.0680     2.0900 ! Butadiene
CG2DC1A   0.0       -0.0680     2.0900 ! Butadiene
CG2DC1B   0.0       -0.0680     2.0900 ! Butadiene
CG2DC1C   0.0       -0.0680     2.0900 ! Butadiene
CG2DC1D   0.0       -0.0680     2.0900 ! Butadiene

!oxygen
OG301    0.0       -0.1000     1.6500 ! ether; LJ from THP, sng 1/06
            !SHOULD WE HAVE A SEPARATE ENOL ETHER??? IF YES, SHOULD WE MERGE IT WITH OG3R60???
```