Supplementary Information for

Drude Polarizable Force Field for Aliphatic Ketones and Aldehydes, and their Associated Acyclic Carbohydrates

Meagan C. Small[†]*, Asaminew H. Aytenfisu*[†]*, Fang-Yu Lin, Xibing He, and*

Alexander D. MacKerell, Jr.[*]

Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, 20 Penn St., Baltimore MD 21201

[†]These authors contributed equally to this work.

*Corresponding author: alex@outerbanks.umaryland.edu

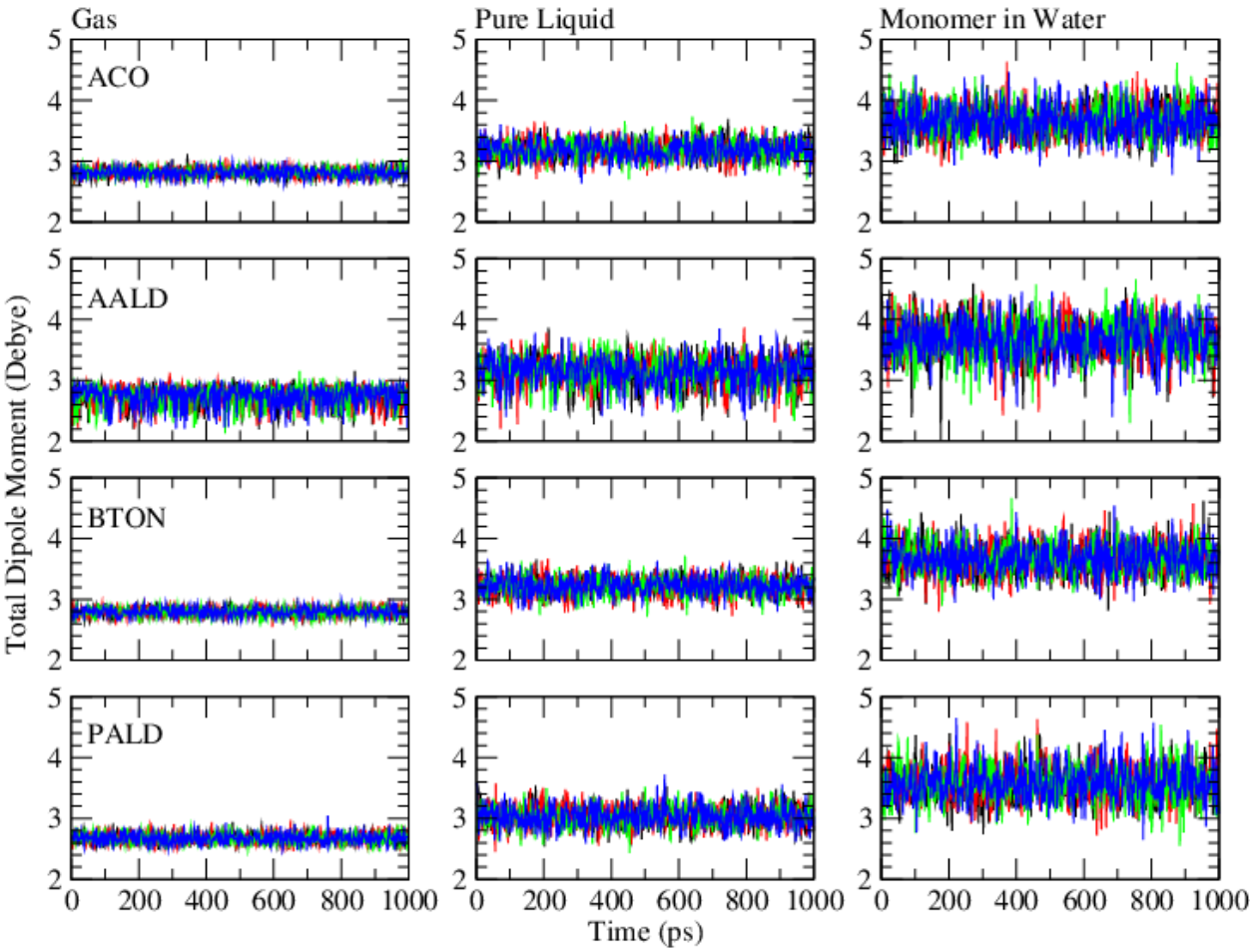

Figure S1 Dipole moments as a function of time for acetone (ACO), acetaldehyde (AALD), butanone (BTON), and propionaldehyde (PALD) in the gas phase (left column), pure liquid (middle column), and aqueous solution (right column). Results from a series of 4 simulations are presented for each system.

Table S1 Select distances (Å) and angles (degrees) for acetone (ACO) from crystal simulations performed using the Drude FF and from the experimental crystal conformation obtained from the CSD ID=HIXHIF03. Averages and standard errors are based on 3 simulations.

CSID:HIXHIF03		Average ± SE
12C2-12C1-12C3 (angle)	**exp**	**117.10**
	drude	116.72 ± 0.06
12O1 ... 9C1 (distance)	**exp**	**3.40**
	drude	3.67 ± 0.00
9C3 ...13C2 (distance)	**exp**	**4.10**
	drude	4.35 ± 0.01
9C3 ... 2C3 (distance)	**exp**	**4.20**
	drude	3.83 ± 0.01

Table S2 Select distances (Å) and angles (degrees) for acetone (ACO) from crystal simulations performed using the Drude FF and from the experimental crystal conformation obtained from the CSD ID=HIXHIF05. Averages and standard errors are based on 3 simulations.

CSID:HIXHIF05		Average ± SE
1C2-1C1-1C3 (angle)	**exp**	**115.70**
	drude	116.84 ± 0.14
1O1 ... 3C1 (distance)	**exp**	**3.20**
	drude	3.63 ± 0.00
1C3 ... 2C2 (distance)	**exp**	**3.50**
	drude	3.37 ± 0.00
1C3 ... 3C3 (distance)	**exp**	**4.30**
	drude	4.27 ± 0.00

Table S3 Select distances (Å) and angles (degrees) for acetone (ACO) from crystal simulations performed using the Drude FF and optimized ACO parameters and from the experimental crystal conformation obtained from the CSD ID=HIXHIF02. Averages and standard errors are based on 3 simulations.

CSID:HIXHIF02		Average ± SE
11C2-11C1-11C3 (angle)	**exp**	**116.30**
	drude	116.68 ± 0.13
11O1 ... 14C1 (distance)	**exp**	**3.50**
	drude	3.69 ± 0.01
10C2 ... 14C3 (distance)	**exp**	**4.20**
	drude	4.39 ± 0.02
1C3 ...14C3(distance)	**exp**	**4.10**
	drude	3.87± 0.01

Table S4 Bond lengths (Å) and angles (degrees) for D-allose and D-psicose from QM optimizations at the MP2/6-31G(d) level of theory and the Drude force field. Only bonds and angles containing the covalent linkage between the polyols and ketone/aldehydes as shown here were optimized.

	Atoms	QM	MM	MM-QM
D-allose	C1-C2	1.51	1.52	0.01
	H1-C1-C2	117.73	116.99	-0.74
	O1-C1-C2	120.04	123.97	3.93
	C1-C2-O2	109.19	112.45	3.26
	C1-C2-H2	109.07	104.42	-4.65
D-psicose	C2-C3	1.52	1.53	0.01
	C1-C2	1.51	1.54	0.03
	H11-C1-C2	108.76	107.95	-0.81
	H12-C1-C2	107.66	108.13	0.47
	C1-C2=O2	119.42	122.01	2.59
	O2=C2-C3	121.68	121.16	-0.52
	C1-C2-C3	118.90	116.78	-2.12
	C2-C3-O3	106.66	110.01	3.35
	C2-C3-H3	106.91	106.08	-0.83
	C2-C3-C4	110.7	113.42	2.72

Table S5 Topology and parameter files for acetone (ACO), butanone (BTON), acetaldehyde (AALD), propionaldehyde (PALD), butaryaldehyde, isobutaryaldehyde, D-allose and D-psicose.

```
* Toppar stream file for drude aliphate aldehyde and
* ketone model compounds
*

ioformat extended

read rtf card append
* Topology for drude model compounds
*
34


AUTOGENERATE ANGLES DIHEDRALS DRUDE

RESI AALD        0.00 ! acetaldehyde
!       O  HB1
!       ||   |
!  HA---C---CB---HB3
!            |
!           HB2
GROUP
ATOM HA    HDP1C   0.011
ATOM C     CD2O1C  0.300    ALPHA -1.1432 THOLE 1.1720
ATOM O     OD2C1C  0.000    ALPHA -0.8125 THOLE 1.2500
ATOM CB    CD33C  -0.088    ALPHA -1.3500 THOLE 1.1500
ATOM HB1   HDA3A   0.056
ATOM HB2   HDA3A   0.056
ATOM HB3   HDA3A   0.056
ATOM LPA   LPD    -0.234
ATOM LPB   LPD    -0.157



BOND HA C   C CB  CB HB1  CB HB2  CB HB3
BOND O  LPA O LPB
DOUB C O
IMPR C HA CB O
ACCE O
LONEPAIR relative LPA O C HA distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPB O C HA distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY       O      C    LPA    LPB  A11  0.85956 A22  1.13122
IC O   C   CB   HB1        1.2074  123.73   -0.46  108.58   1.1053
IC HB2 CB  C    O          1.0625  110.65  118.23  123.73   1.2074
IC HB3 CB  C    O          1.0898  105.98 -126.83  123.73   1.2074
IC HA  O   *C   CB         1.1347  126.86 -176.51  123.73   1.5462
PATCHING FIRST NONE LAST NONE

RESI PALD        0.00 ! propionaldehyde
!       O  HB1  HG1
!       ||   |    |
```

```
!  HA---C---CB---CG---HG3
!            |    |
!           HB2  HG2
GROUP
ATOM HA    HDP1C   0.011
ATOM C     CD2O1C  0.300    ALPHA -1.1432 THOLE 1.1720
ATOM O     OD2C1C  0.000    ALPHA -0.8125 THOLE 1.2500
ATOM CB    CD32C  -0.088    ALPHA -1.3500 THOLE 1.1500
ATOM HB1   HDA2A   0.056
ATOM HB2   HDA2A   0.056
ATOM LPA   LPD    -0.234
ATOM LPB   LPD    -0.157
ATOM CG    CD33A  -0.064    ALPHA -1.254 THOLE 1.779
ATOM HG1   HDA3A   0.040
ATOM HG2   HDA3A   0.040
ATOM HG3   HDA3A   0.040

BOND HA C   C CB   CB HB1  CB HB2
BOND CB CG  CG HG1 CG HG3  CG HG2
BOND O  LPA O LPB
DOUBLE C O
IMPR C HA CB O
ACCE O
LONEPAIR relative LPA O C HA distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPB O C HA distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY       O      C    LPA    LPB  A11  0.85956 A22  1.13122
IC O C CB CG        0.0     0.0     0.0      0.0   0.0
IC CG CB C HA       0.0     0.0   180.0      0.0   0.0
IC HB1 CB C O       0.0     0.0   120.0      0.0   0.0
IC HB2 CB C O       0.0     0.0  -120.0      0.0   0.0
IC C CB CG HG1      0.0     0.0   180.0      0.0   0.0
IC C CB CG HG2      0.0     0.0    60.0      0.0   0.0
IC C CB CG HG3      0.0     0.0   -60.0      0.0   0.0
PATCHING FIRST NONE LAST NONE

RESI BALD        0.00 ! Butaryaldehyde
!       O  HB1  HG1   HF1
!       ||   |    |    |
!  HA---C---CB---CG---CF---HF3
!            |    |    |
!           HB2  HG2  HF2

GROUP
ATOM HA    HDP1C   0.011
ATOM C     CD2O1C  0.300    ALPHA -1.1432  THOLE 1.1720
ATOM O     OD2C1C  0.000    ALPHA -0.8125  THOLE 1.2500
ATOM CB    CD32C  -0.088    ALPHA -1.3500  THOLE 1.1500
ATOM HB1   HDA2A   0.056
ATOM HB2   HDA2A   0.056
ATOM LPA   LPD    -0.234
ATOM LPB   LPD    -0.157
ATOM CG    CD32A  -0.080   ALPHA -1.254 THOLE 1.779
ATOM HG1   HDA2A   0.040
ATOM HG2   HDA2A   0.040
```

```
ATOM CF    CD33A  -0.064   ALPHA -1.254 THOLE 1.779
ATOM HF1   HDA3A   0.040
ATOM HF2   HDA3A   0.040
ATOM HF3   HDA3A   0.040

BOND HA C    C CB   CB HB1  CB HB2
BOND CB CG   CG HG1    CG HG2     CG CF    CF HF1   CF HF2    CF HF3
BOND O  LPA O LPB
DOUBLE C O
IMPR C HA CB O
ACCE O
LONEPAIR relative LPA O C HA distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPB O C HA distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY       O      C    LPA    LPB  A11  0.85956 A22  1.13122
IC O C CB CG        0.0     0.0     0.0      0.0   0.0
IC CG CB C HA       0.0     0.0   180.0      0.0   0.0
IC HB1 CB C O       0.0     0.0   120.0      0.0   0.0
IC HB2 CB C O       0.0     0.0  -120.0      0.0   0.0
IC C CB CG HG1      0.0     0.0   180.0      0.0   0.0
IC C CB CG HG2      0.0     0.0    60.0      0.0   0.0
IC C CB CG CF       0.0     0.0   -60.0      0.0   0.0

IC CB CG CF HF1     0.0     0.0  -180.0      0.0   0.0
IC CB CG CF HF2     0.0     0.0    60.0      0.0   0.0
IC CB CG CF HF3     0.0     0.0   -60.0      0.0   0.0

PATCHING FIRST NONE LAST NONE

RESI IBLD        0.00 ! Isobutaryaldehyde
!       O    HB1 HF1
!       ||   |    |
!  HA---C---CB---CF---HF2
!           |    |
!      HG1---CG  HF3
!           / \
!        HG2  HG3
GROUP
ATOM HA    HDP1C   0.011
ATOM C     CD2O1C  0.300    ALPHA -1.1432 THOLE 1.1720
ATOM O     OD2C1C  0.000    ALPHA -0.8125 THOLE 1.2500
ATOM CB    CD31C  -0.088    ALPHA -1.3500 THOLE 1.1500
ATOM HB1   HDA1A   0.056
ATOM LPA   LPD    -0.234
ATOM LPB   LPD    -0.157
ATOM CG    CD33A  -0.064    ALPHA -1.254 THOLE 1.779
ATOM HG1   HDA3A   0.040
ATOM HG2   HDA3A   0.040
ATOM HG3   HDA3A   0.040
ATOM CF    CD33A  -0.064   ALPHA -1.254 THOLE 1.779
ATOM HF1   HDA3A   0.040
ATOM HF2   HDA3A   0.040
ATOM HF3   HDA3A   0.040

BOND HA C   C CB   CB HB1
BOND CB CG  CG HG1 CG HG2 CG HG3
```

```
BOND CB CF  CF HF1 CF HF2 CF HF3
BOND O  LPA O LPB
DOUBLE C O
IMPR C HA CB O
ACCE O
LONEPAIR relative LPA O C HA distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPB O C HA distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY       O      C    LPA    LPB  A11  0.85956 A22  1.13122
IC O    C  CB CG      0.0     0.0     0.0      0.0   0.0
IC CG   CB C  HA      0.0     0.0   180.0      0.0   0.0
IC HB1  CB C  O       0.0     0.0   120.0      0.0   0.0
IC CF  CB C  O       0.0     0.0  -120.0      0.0   0.0
IC C    CB CG HG1     0.0     0.0   180.0      0.0   0.0
IC C    CB CG HG2     0.0     0.0    60.0      0.0   0.0
IC C    CB CG HG3     0.0     0.0   -60.0      0.0   0.0
IC C    CB CF HF1     0.0     0.0   180.0      0.0   0.0
IC C    CB CF HF2     0.0     0.0    60.0      0.0   0.0
IC C    CB CF HF3     0.0     0.0   -60.0      0.0   0.0


PATCHING FIRST NONE LAST NONE

RESI ACO 0.0  ! acetone
!      H22  O1  H32
!       |   ||   |
!   H21-C2--C1--C3-H31
!       |        |
!      H23      H33

GROUP
ATOM O1     OD2C1D    0.000   ALPHA -0.638  THOLE 1.426
ATOM C1     CD2O1D    0.486   ALPHA -1.154  THOLE 1.235
ATOM C2     CD33C    -0.201   ALPHA -1.293  THOLE 1.181
ATOM H21    HDA3A     0.062
ATOM H22    HDA3A     0.062
ATOM H23    HDA3A     0.062
ATOM C3     CD33C    -0.201   ALPHA -1.293  THOLE 1.181
ATOM H31    HDA3A     0.062
ATOM H32    HDA3A     0.062
ATOM H33    HDA3A     0.062
ATOM LPA    LPD      -0.228
ATOM LPB    LPD      -0.228

BOND    C1 C2   C1 C3
BOND    C2 H21  C2 H22   C2 H23
BOND    C3 H31  C3 H32   C3 H33
BOND    O1 LPA O1 LPB
DOUBLE  O1 C1
IMPR    C1 C2 C3 O1
ACCE    O1
!from NMA
LONEPAIR relative LPA O1 C1 C2 distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPB O1 C1 C2 distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY       O1      C1    LPA    LPB  A11  0.86650 A22  1.07246
IC C2   C1   C3  H31        1.5366  110.58  135.22  109.51   1.1328
```

```
IC O1   C1   C3  H31        1.2237  122.95  -42.47  109.51   1.1328
IC O1   C1   C3  H32        1.2237  122.95   77.28  104.63   1.1325
IC O1   C1   C3  H33        1.2237  122.95 -161.85  105.76   1.0732
IC C3   C1   C2  H21        1.5233  110.58 -153.74  111.52   1.1204
IC O1   C1   C2  H21        1.2237  126.42   23.85  111.52   1.1204
IC O1   C1   C2  H22        1.2237  126.42  148.26  114.11   1.1296
IC O1   C1   C2  H23        1.2237  126.42  -90.21  101.67   1.1375
PATCHING FIRST NONE LAST NONE

RESI BTON 0.0  ! 2-butanone
!      H22  O1  H32 H42
!       |   ||   |   |
!   H23-C2--C1--C3--C4-H43
!       |        |   |
!      H21      H31 H41
GROUP
ATOM O1     OD2C1D    0.000   ALPHA -0.638  THOLE 1.426
ATOM C1     CD2O1D    0.486   ALPHA -1.154  THOLE 1.235
ATOM C2     CD33C    -0.201   ALPHA -1.293  THOLE 1.181
ATOM C3     CD32C    -0.139   ALPHA -1.293  THOLE 1.181
ATOM H21    HDA3A     0.062
ATOM H22    HDA3A     0.062
ATOM H23    HDA3A     0.062
ATOM H31    HDA2A     0.062
ATOM H32    HDA2A     0.062
ATOM LPA    LPD      -0.228
ATOM LPB    LPD      -0.228
ATOM C4     CD33A    -0.177  ALPHA -1.751 THOLE 1.185
ATOM H41    HDA3A     0.059
ATOM H42    HDA3A     0.059
ATOM H43    HDA3A     0.059

BOND    C1 C2   C1 C3    C3 C4
BOND    C2 H21  C2 H22   C2 H23
BOND    C3 H31  C3 H32
BOND    C4 H41  C4 H42   C4 H43
BOND    O1 LPA  O1 LPB
DOUBLE  O1 C1
IMPR    C1 C2 C3 O1
ACCE    O1
!from NMA
LONEPAIR relative LPA O1 C1 C2 distance 0.30 angle 91.0 dihe 0.0
LONEPAIR relative LPB O1 C1 C2 distance 0.30 angle 91.0 dihe 180.0
ANISOTROPY       O1      C1    LPA    LPB  A11  0.86650 A22  1.07246
IC C2   C1   C3  H31        1.5366  116.31   56.91  107.51   1.1328
IC O1   C1   C3  H31        1.2237  122.02 -123.36  107.51   1.1328
IC O1   C1   C3  H32        1.2237  122.02  124.49  107.48   1.1325
IC C3   C1   C2  H21        1.5233  110.58 -153.74  111.52   1.1204
IC O1   C1   C2  H21        1.2237  126.42   23.85  111.52   1.1204
IC O1   C1   C2  H22        1.2237  126.42  148.26  114.11   1.1296
IC O1   C1   C2  H23        1.2237  126.42  -90.21  101.67   1.1375
IC O1   C1   C3  C4         1.2237  122.02    0.50  114.19   1.5261
IC C2   C1   C3  C4         1.5366  116.31 -179.21  114.19   1.5261
IC C1   C3   C4  H41        1.5233  114.19  -60.64  111.01   1.0980
IC C1   C3   C4  H42        1.5233  114.19  178.91  110.72   1.0989
```

```
IC C1   C3   C4  H43        1.5233  114.19   58.43  111.02   1.0980
PATCHING FIRST NONE LAST NONE

!carbonyl containing acyclic sugars

RESI ALLO       0.000 ! D-allose
!          HA    O1
!            \  //
!             C1     transferred from AALD
!             |
!      HO2-O2-C2-H2
!             |
!      HO3-O3-C3-H3
!             |
!      HO4-O4-C4-H4
!             |
!      HO5-O5-C5-H5
!             |
!         H61-C6-H62
!             |
!             O6-HO6
!
GROUP
ATOM H1   HDP1C    0.011
ATOM C1   CD2O1C   0.3  ALPHA -1.1432  THOLE 1.1720
ATOM O1   OD2C1C   0.000  ALPHA -0.8125  THOLE 1.2500
ATOM LP1A LPD     -0.234
ATOM LP1B LPD     -0.157
ATOM C2   CD31G    0.090  ALPHA -1.650  THOLE 0.700
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO2  HDP1A    0.320
ATOM LP2A LPD     -0.200
ATOM LP2B LPD     -0.200
GROUP
ATOM C3   CD31G    0.010  ALPHA -1.650  THOLE 0.700
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO3  HDP1A    0.320
ATOM LP3A LPD     -0.200
ATOM LP3B LPD     -0.200
GROUP
ATOM C4   CD31G    0.010  ALPHA -1.650  THOLE 0.700
ATOM H4   HDA1A    0.070
ATOM O4   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO4  HDP1A    0.320
ATOM LP4A LPD     -0.200
ATOM LP4B LPD     -0.200
GROUP
ATOM C5   CD31G    0.010  ALPHA -1.650  THOLE 0.700
ATOM H5   HDA1A    0.070
ATOM O5   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO5  HDP1A    0.320
ATOM LP5A LPD     -0.200
ATOM LP5B LPD     -0.200
```

```
GROUP
ATOM C6   CD32F   -0.060  ALPHA -1.650  THOLE 0.700
ATOM H61  HDA2A    0.070
ATOM H62  HDA2A    0.070
ATOM O6   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO6  HDP1A    0.320
ATOM LP6A LPD     -0.200
ATOM LP6B LPD     -0.200

BOND C1 H1   C1 O1    C1 C2
BOND C2 H2   C2 C3    C2 O2    O2 HO2
BOND C3 H3   C3 C4    C3 O3    O3 HO3
BOND C4 H4   C4 O4    C4 C5    O4 HO4
BOND C5 H5   C5 O5    C5 C6    O5 HO5
BOND C6 H61  C6 O6    C6 H62   O6 HO6
BOND O1 LP1A   O1 LP1B
BOND O2 LP2A   O2 LP2B
BOND O3 LP3A   O3 LP3B
BOND O4 LP4A   O4 LP4B
BOND O5 LP5A   O5 LP5B
BOND O6 LP6A   O6 LP6B
IMPR C1 H1 C2 O1

LONEPAIR relative LP1A O1 C1 H1  distance 0.30 angle  91.0 dihe   0.0
LONEPAIR relative LP1B O1 C1 H1  distance 0.30 angle  91.0 dihe 180.0
LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP4A O4 C4 HO4 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP4B O4 C4 HO4 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP6A O6 C6 HO6 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP6B O6 C6 HO6 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.85956 A22 1.13122
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108  A22 1.2162
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108  A22 1.2162
ANISOTROPY O4 C4 LP4A LP4B A11 0.8108  A22 1.2162
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108  A22 1.2162
ANISOTROPY O6 C6 LP6A LP6B A11 0.8108  A22 1.2162

!    I    J    K    L      R(IK)   T(IKJ)    PHI   T(JKL)   R(KL)
IC   C1   C2   C3   C4     1.6170  111.59  180.00  110.42   1.5369
IC   C2   C3   C4   C5     1.5300  110.42  180.00  110.20   1.5320
IC   C3   C4   C5   C6     1.5369  110.20  180.00  108.72   1.5316
IC   C3   C2   C1   O1     1.5000  113.80  180.00  124.00   1.2050
IC   O1   C2   *C1  H1     1.4350  108.07  180.00  105.35   1.0997
IC   C3   C1   *C2  O2     1.5300  111.59  120.00  109.42   1.4226
IC   C3   C1   *C2  H2     1.4226  109.42 -120.00  109.09   1.1814
IC   C1   C2   O2   HO2    1.6170  109.42  -60.00   99.72   0.9669
IC   C4   C2   *C3  O3     1.5369  110.42  120.00  111.02   1.4276
IC   C4   C2   *C3  H3     1.4276  111.02 -120.00  106.54   1.1878
IC   C2   C3   O3   HO3    1.5300  111.02  -60.00   98.73   0.9915
IC   C5   C3   *C4  O4     1.5320  110.20  120.00  112.07   1.3955
```

```
IC   C5   C3   *C4  H4     1.3955  112.07 -120.00  113.60   1.0969
IC   C3   C4   O4   HO4    1.5369  112.07  -60.00  103.63   0.9940
IC   C6   C4   *C5  O5     1.5316  108.72  120.00  111.89   1.3976
IC   C6   C4   *C5  H5     1.5316  108.72 -120.00  105.82   1.1468
IC   C4   C5   O5   HO5    1.5320  111.89  -60.00  105.13   0.9258
IC   C4   C5   C6   O6     1.5320  108.72  180.00  105.74   1.4909
IC   O6   C5   *C6  H61    1.4909  105.74  120.00  106.59   1.0511
IC   O6   C5   *C6  H62    1.0511  106.59 -120.00  106.23   1.0677
IC   C5   C6   O6   HO6    1.5316  105.74  180.00  115.02   0.9350
PATC FIRS NONE LAST NONE


RESI PSIC       0.000 ! D-psicose
!             O1-HO1
!              |
!         H11-C1-H12
!              |
!              C2=O2
!              |
!      HO3-O3-C3-H3
!              |
!      HO4-O4-C4-H4
!              |
!      HO5-O5-C5-H5
!              |
!         H61-C6-H62
!              |
!              O6-HO6
!
GROUP
ATOM C1   CD32F   -0.090  ALPHA -1.650  THOLE 0.700
ATOM H11  HDA2A    0.070
ATOM H12  HDA2A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO1  HDP1A    0.320
ATOM LP1A LPD     -0.200
ATOM LP1B LPD     -0.200
ATOM C2   CD2O1D   0.486  ALPHA -1.154  THOLE 1.235
ATOM O2   OD2C1D   0.000  ALPHA -0.638  THOLE 1.426
ATOM LP2A LPD     -0.228
ATOM LP2B LPD     -0.228
GROUP
ATOM C3   CD31G    0.010  ALPHA -1.650  THOLE 0.700
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO3  HDP1A    0.320
ATOM LP3A LPD     -0.200
ATOM LP3B LPD     -0.200
GROUP
ATOM C4   CD31G    0.010  ALPHA -1.650  THOLE 0.700
ATOM H4   HDA1A    0.070
ATOM O4   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO4  HDP1A    0.320
ATOM LP4A LPD     -0.200
ATOM LP4B LPD     -0.200
```

```
GROUP
ATOM C5   CD31G    0.010  ALPHA -1.650  THOLE 0.700
ATOM H5   HDA1A    0.070
ATOM O5   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO5  HDP1A    0.320
ATOM LP5A LPD     -0.200
ATOM LP5B LPD     -0.200
GROUP
ATOM C6   CD32F   -0.060  ALPHA -1.650  THOLE 0.700
ATOM H61  HDA2A    0.070
ATOM H62  HDA2A    0.070
ATOM O6   OD31E    0.000  ALPHA -1.000  THOLE 1.000
ATOM HO6  HDP1A    0.320
ATOM LP6A LPD     -0.200
ATOM LP6B LPD     -0.200

BOND C1   O1        C1   H11       O1   HO1       C1   H12       C1   C2
BOND C2   O2        C2   C3        C3   H3
BOND C3   O3        O3   HO3       C3   C4        C4   H4        C4   O4
BOND O4   HO4       C4   C5        C5   H5        C5   C6        C6   H61
BOND C6   H62       C6   O6        O6   HO6       C5   O5        O5   HO5
BOND O1 LP1A   O1 LP1B
BOND O2 LP2A   O2 LP2B
BOND O3 LP3A   O3 LP3B
BOND O4 LP4A   O4 LP4B
BOND O5 LP5A   O5 LP5B
BOND O6 LP6A   O6 LP6B
IMPR C2  C1  C3  O2

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP2A O2 C2 C1  distance 0.30 angle  91.0 dihe   0.0
LONEPAIR relative LP2B O2 C2 C1  distance 0.30 angle  91.0 dihe 180.0
LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP4A O4 C4 HO4 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP4B O4 C4 HO4 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
LONEPAIR relative LP6A O6 C6 HO6 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP6B O6 C6 HO6 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108  A22 1.2162
ANISOTROPY O2 C2 LP2A LP2B A11 0.8665  A22 1.07246
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108  A22 1.2162
ANISOTROPY O4 C4 LP4A LP4B A11 0.8108  A22 1.2162
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108  A22 1.2162
ANISOTROPY O6 C6 LP6A LP6B A11 0.8108  A22 1.2162

!    I    J    K    L      R(IK)   T(IKJ)    PHI   T(JKL)   R(KL)
IC   C1   C2   C3   C4     1.6170  111.59  180.00  110.42   1.5369
IC   C2   C3   C4   C5     1.5300  110.42  180.00  110.20   1.5320
IC   C3   C4   C5   C6     1.5369  110.20  180.00  108.72   1.5316
IC   C3   C2   C1   O1     1.5000  116.00  180.00  108.89   1.4200
IC   C2   C1   O1   HO1    1.6170  108.07  180.00  109.97   0.9462
IC   O1   C2   *C1  H11    1.4350  108.07  120.00  105.35   1.0997
```

```
IC   O1   C2   *C1  H12    1.4350  108.07 -120.00  109.50   1.1112
IC   O1   C2   *C1  H1     1.4350  108.07  180.00  105.35   1.0997
IC   C3   C1   *C2  O2     1.5300  111.59  180.00  109.42   1.4226
IC   C4   C2   *C3  O3     1.5369  110.42  120.00  111.02   1.4276
IC   C4   C2   *C3  H3     1.4276  111.02 -120.00  106.54   1.1878
IC   C2   C3   O3   HO3    1.5300  111.02  -60.00   98.73   0.9915
IC   C5   C3   *C4  O4     1.5320  110.20  120.00  112.07   1.3955
IC   C5   C3   *C4  H4     1.3955  112.07 -120.00  113.60   1.0969
IC   C3   C4   O4   HO4    1.5369  112.07  -60.00  103.63   0.9940
IC   C6   C4   *C5  O5     1.5316  108.72  120.00  111.89   1.3976
IC   C6   C4   *C5  H5     1.5316  108.72 -120.00  105.82   1.1468 !
IC   C4   C5   O5   HO5    1.5320  111.89  -60.00  105.13   0.9258
IC   C4   C5   C6   O6     1.5320  108.72  180.00  105.74   1.4909
IC   O6   C5   *C6  H61    1.4909  105.74  120.00  106.59   1.0511
IC   O6   C5   *C6  H62    1.0511  106.59 -120.00  106.23   1.0677
IC   C5   C6   O6   HO6    1.5316  105.74  180.00  115.02   0.9350


END

read para card append
* Drude polarizable FF parameters, aldehydes and ketones
*


BONDS

CD2O1C   CD31C    245.00      1.491 !
CD2O1D   LPD        0.00      0.000 !
CD2O1C   LPD        0.00      0.000 !
OD2C1D   LPD        0.00      0.000 !
OD2C1C   LPD        0.00      0.000 !
OD2C1D   CD2O1D   750.00      1.218 !
CD2O1D   CD33C    250.00      1.498 !
CD2O1D   CD32C    245.00      1.491 !
CD2O1C   HDP1C    310.00      1.104 !
OD2C1C   CD2O1C   750.00      1.218 !
CD2O1C   CD33C    250.00      1.498 !
CD2O1C   CD32C    245.00      1.491 !
CD2O1C   CD31G    245.00      1.491 !
CD2O1D   CD32F    250.00      1.498 !
CD2O1D   CD31G    245.00      1.491 !
OD31E    HDP1A    536.50      0.960 !
OD31E    CD32F    320.00      1.425 !
OD31E    CD31G    350.00      1.430 !
CD32F    CD32F    222.50      1.500 !
CD32F    CD31G    222.50      1.510 !
CD31G    CD31G    222.50      1.510 !
CD32F    HDA2A    309.00      1.080 !
CD31G    HDA1A    309.00      1.080 !
OD31E    LPD        0.00      0.000 !
CD32F    LPD        0.00      0.000 !
CD31G    LPD        0.00      0.000 !
!!!!!!!!!!!!
```

```
ANGLES
CD2O1D   CD33C    HDA3A     38.70    109.30 !
OD2C1D   CD2O1D   CD33C     63.60    121.81 !
CD33C    CD2O1D   CD33C     44.50    116.38 !
OD2C1D   CD2O1D   CD32C     60.60    121.19 !
CD33C    CD2O1D   CD32C     47.60    117.00 !
CD2O1D   CD32C    CD33A     55.40    110.90 !
CD2O1D   CD32C    HDA2A     39.00    107.77 !
CD2O1D   CD32C    CD32A     57.50    110.20 !
CD32C    CD2O1D   CD32C     52.50    117.80 !
OD2C1D   CD2O1C   HDP1C     55.5     118.00 !
OD2C1C   CD2O1C   HDP1C     55.5     118.00 !
HDP1C    CD2O1C   CD33C     20.00    115.30 !
CD2O1C   CD33C    HDA3A     38.70    109.30 !
OD2C1C   CD2O1C   CD33C     63.60    123.81 !
OD2C1C   CD2O1C   CD32C     60.60    121.19 !
OD2C1C   CD2O1C   CD31C     60.60    121.19 !
CD2O1C   CD32C    CD33A     55.40    110.90 !
CD2O1C   CD32C    HDA2A     39.00    107.77 !
CD2O1C   CD32C    CD32A     57.50    110.20 !
CD2O1C   CD31C    CD33A     55.40    110.90 !
CD2O1C   CD31C    HDA1A     39.00    107.77 !
CD33A    CD31C    CD33A     58.35    113.50   11.16   2.561 !
HDP1C    CD2O1C   CD32C     30.0     115.22 !
HDP1C    CD2O1C   CD31C     30.0     115.22 !
!!!!!!!!!!!!!!!!!!!
HDA2A    CD32F    CD2O1D    26.50    110.10   22.53   2.179  !
OD31E    CD32F    CD2O1D    66.00    111.00 !
CD32F    CD2O1D   OD2C1D    63.60    121.81 !
CD32F    CD2O1D   CD31G     44.50    116.38 !
OD2C1D   CD2O1D   CD31G     63.60    121.81 !
CD2O1D   CD31G    CD31G     55.40    110.90 !
CD2O1D   CD31G    HDA1A     39.00    107.77 !
CD2O1D   CD31G    OD31E     39.00    107.77 !
HDP1C    CD2O1C   CD31G     30.0     115.22 !
OD2C1C   CD2O1C   CD31G     30.0     115.22 !
CD2O1C   CD31G    OD31E     39.00    107.77 !
CD2O1C   CD31G    HDA1A     39.00    107.77 !
CD2O1C   CD31G    CD31G     58.35    113.50   11.16   2.561 !
!
CD31G    OD31E    HDP1A     59.00    108.00 !
CD32F    OD31E    HDP1A     49.00    107.30 !
OD31E    CD31G    CD32F     59.30    111.00 !
OD31E    CD32F    CD31G     66.00    111.00 !
OD31E    CD32F    CD32F     66.00    111.00 !
OD31E    CD31G    CD31G     66.00    111.00 !
OD31E    CD32F    HDA2A     54.00    110.50 !
OD31E    CD31G    HDA1A     47.00    110.50 !
CD32F    CD31G    CD31G     58.35    113.50   11.16   2.561  !
CD32F    CD31G    CD32F     58.35    113.50   11.16   2.561  !
CD31G    CD31G    CD31G     58.35    113.50   11.16   2.561  !
CD31G    CD32F    HDA2A     26.50    110.10   22.53   2.179  !
CD32F    CD31G    HDA1A     34.50    110.10   22.53   2.179  !
CD31G    CD31G    HDA1A     34.50    110.10   22.53   2.179  !
HDA2A    CD32F    HDA2A     35.50    109.00    5.40   1.802  !
```

```
DIHEDRALS
CD33A    CD31C    CD33A    HDA3A       0.150    3     0.00 !
CD2O1C   CD31C    CD33A    HDA3A       0.200    3     0.00 ! CNEU
HDP1C    CD2O1C   CD31C    HDA1A       0.200    3     0.00 !
OD2C1C   CD2O1C   CD31C    HDA1A       0.085    3     0.00 !
CD33C    CD2O1D   CD33C    HDA3A       0.200    3     0.00 ! acetone
CD32C    CD2O1D   CD33C    HDA3A       0.200    3     0.00 !
CD32C    CD2O1D   CD32C    HDA2A       0.200    3     0.00 ! 3-pentanone
CD33C    CD2O1D   CD32C    HDA2A       0.200    3     0.00 !
OD2C1D   CD2O1D   CD33C    HDA3A       0.085    3     0.00 !
OD2C1D   CD2O1D   CD32C    HDA2A       0.085    3     0.00 !
CD2O1D   CD32C    CD33A    HDA3A       0.120    3   180.00 !
CD2O1D   CD32C    CD32A    HDA2A       0.200    3   180.00 !2-pentanone
HDP1C    CD2O1C   CD32C    HDA2A       0.200    3     0.00 ! ethanal
HDP1C    CD2O1C   CD33C    HDA3A       0.200    3     0.00 !
CD2O1C   CD32C    CD33A    HDA3A       0.120    3   180.00 !
CD33A    CD32A    CD32C    CD2O1C      0.5501   1     0.00 !
CD33A    CD32A    CD32C    CD2O1C      0.9806   2     0.00 !
CD33A    CD32A    CD32C    CD2O1C      0.3445   3     0.00 !
CD2O1C   CD32C    CD32A    HDA2A       0.200    3   180.00 !
OD2C1C   CD2O1C   CD33C    HDA3A       0.015    3     0.00 !
OD2C1C   CD2O1C   CD32C    HDA2A       0.015    3     0.00 !
CD2O1C   CD31G    CD31G    HDA1A       0.5750   1     0.00 !
CD2O1C   CD31G    CD31G    HDA1A       0.4780   2     0.00 !
CD2O1C   CD31G    CD31G    HDA1A       0.2480   3     0.00 !
CD2O1C   CD31G    CD31G    OD31E       0.3100   1     0.00 !
CD2O1C   CD31G    CD31G    OD31E       0.1370   2     0.00 !
CD2O1C   CD31G    CD31G    OD31E       0.1130   3     0.00 !
CD2O1C   CD31G    CD31G    CD31G       1.5480   1   180.00 !
CD2O1C   CD31G    CD31G    CD31G       0.3290   2   180.00 !
CD2O1C   CD31G    CD31G    CD31G       0.0960   3   180.00 !
HDP1A    OD31E    CD31G    HDA1A       0.200    3     0.00 !
CD31G    CD31G    OD31E    HDP1A       0.5750   1     0.00 !
CD31G    CD31G    OD31E    HDP1A       0.4780   2     0.00 !
CD31G    CD31G    OD31E    HDP1A       0.2480   3     0.00 !
CD2O1D   CD31G    CD31G    CD31G       1.5480   1   180.00 !
CD2O1D   CD31G    CD31G    CD31G       0.3290   2   180.00 !
CD2O1D   CD31G    CD31G    CD31G       0.0960   3   180.00 !
CD2O1D   CD31G    CD31G    HDA1A       0.200    3     0.00 !
CD2O1D   CD31G    CD31G    OD31E       0.3100   1     0.00 !
CD2O1D   CD31G    CD31G    OD31E       0.1370   2     0.00 !
CD2O1D   CD31G    CD31G    OD31E       0.1130   3     0.00 !
HDP1A    OD31E    CD32F    HDA2A        0.200   3     0.00 !
CD2O1D   CD32F    OD31E    HDP1A        0.5750  1     0.00 !
CD2O1D   CD32F    OD31E    HDP1A        0.4780  2     0.00 !
CD2O1D   CD32F    OD31E    HDP1A        0.2480  3     0.00 !
CD2O1D   CD31G    OD31E    HDP1A        0.5750  1     0.00 !
CD2O1D   CD31G    OD31E    HDP1A        0.4780  2     0.00 !
CD2O1D   CD31G    OD31E    HDP1A        0.2480  3     0.00 !
CD31G    CD31G    CD31G    OD31E        0.3100  1     0.00 !
CD31G    CD31G    CD31G    OD31E        0.1370  2     0.00 !
CD31G    CD31G    CD31G    OD31E        0.1130  3     0.00 !
CD31G    CD31G    CD31G    CD31G        1.5480  1   180.00 !
CD31G    CD31G    CD31G    CD31G        0.3290  2   180.00 !
```

```
CD31G    CD31G    CD31G    CD31G        0.0960  3   180.00 !
HDA1A    CD31G    CD31G    HDA1A        0.200   3     0.00 !
HDA1A    CD31G    CD31G    CD31G        0.200   3     0.00 !
OD31E    CD31G    CD31G    HDA1A        0.200   3     0.00 !
OD31E    CD31G    CD31G    OD31E        1.3050  1   180.00 !
OD31E    CD31G    CD31G    OD31E        0.3760  2   180.00 !
OD31E    CD31G    CD31G    OD31E        0.4130  3   180.00 !
CD31G    CD31G    CD31G    CD32F        1.5480  1   180.00 !
CD31G    CD31G    CD31G    CD32F        0.3290  2   180.00 !
CD31G    CD31G    CD31G    CD32F        0.0960  3   180.00 !
CD31G    CD31G    CD32F    OD31E        0.3100  1     0.00 !
CD31G    CD31G    CD32F    OD31E        0.1370  2     0.00 !
CD31G    CD31G    CD32F    OD31E        0.1130  3     0.00 !
HDA1A    CD31G    CD31G    CD32F        0.200   3     0.00 !
CD31G    CD32F    OD31E    HDP1A        0.5750  1     0.00 !
CD31G    CD32F    OD31E    HDP1A        0.4780  2     0.00 !
CD31G    CD32F    OD31E    HDP1A        0.2480  3     0.00 !
OD31E    CD31G    CD32F    HDA2A        0.200   3     0.00 ! glycerol, xhe
OD31E    CD31G    CD32F    OD31E        1.3050  1   180.00 !
OD31E    CD31G    CD32F    OD31E        0.3760  2   180.00 !
OD31E    CD31G    CD32F    OD31E        0.4130  3   180.00 !
HDA2A    CD32F    CD31G    CD31G        0.200   3     0.00 !
CD32F    CD31G    CD31G    OD31E        0.3100  1     0.00 !
CD32F    CD31G    CD31G    OD31E        0.1370  2     0.00 !
CD32F    CD31G    CD31G    OD31E        0.1130  3     0.00 !
HDA2A    CD32F    CD31G    HDA1A        0.200   3     0.00 ! glycerol, xhe
OD31E    CD32F    CD31G    HDA1A        0.200   3     0.00 ! glycerol, xhe
CD32F    CD31G    OD31E    HDP1A        0.5750  1     0.00 !
CD32F    CD31G    OD31E    HDP1A        0.4780  2     0.00 !
CD32F    CD31G    OD31E    HDP1A        0.2480  3     0.00 !
!bton
CD33C    CD2O1D   CD32C    CD33A        0.3865  1     0.00 !
CD33C    CD2O1D   CD32C    CD33A        0.1195  2   180.00 !
CD33C    CD2O1D   CD32C    CD33A        0.0911  3     0.00 !
CD33C    CD2O1D   CD32C    CD33A        0.0307  6     0.00 !
OD2C1D   CD2O1D   CD32C    CD33A        0.3890  1   180.00 !
OD2C1D   CD2O1D   CD32C    CD33A        0.2715  2   180.00 !
OD2C1D   CD2O1D   CD32C    CD33A        0.0825  3   180.00 !
OD2C1D   CD2O1D   CD32C    CD33A        0.0164  6     0.00 !
!pald
OD2C1C   CD2O1C   CD32C    CD33A        0.2416  1   180.00 !
OD2C1C   CD2O1C   CD32C    CD33A        0.2059  2   180.00 !
OD2C1C   CD2O1C   CD32C    CD33A        0.1496  3   180.00 !
OD2C1C   CD2O1C   CD32C    CD33A        0.0765  6   180.00 !
HDP1C    CD2O1C   CD32C    CD33A        0.2240  1     0.00 !
HDP1C    CD2O1C   CD32C    CD33A        0.2179  2   180.00 !
HDP1C    CD2O1C   CD32C    CD33A        0.3116  3     0.00 !
HDP1C    CD2O1C   CD32C    CD33A        0.0606  6     0.00 !
!bald
OD2C1C   CD2O1C   CD32C    CD32A        0.3296  1   180.00 !
OD2C1C   CD2O1C   CD32C    CD32A        0.1850  2   180.00 !
OD2C1C   CD2O1C   CD32C    CD32A        0.1420  3   180.00 !
OD2C1C   CD2O1C   CD32C    CD32A        0.0086  6     0.00 !
HDP1C    CD2O1C   CD32C    CD32A        0.2032  1     0.00 !
HDP1C    CD2O1C   CD32C    CD32A        0.0704  2   180.00 !
```

```
HDP1C    CD2O1C   CD32C    CD32A        0.2642  3     0.00 !
HDP1C    CD2O1C   CD32C    CD32A        0.0220  6   180.00 !
!ibld
OD2C1C   CD2O1C   CD31C    CD33A        0.3499  1   180.00 !
OD2C1C   CD2O1C   CD31C    CD33A        0.4616  2   180.00 !
OD2C1C   CD2O1C   CD31C    CD33A        0.3495  3   180.00 !
OD2C1C   CD2O1C   CD31C    CD33A        0.0181  6     0.00 !
HDP1C    CD2O1C   CD31C    CD33A        0.0438  1   180.00 !
HDP1C    CD2O1C   CD31C    CD33A        0.0154  2   180.00 !
HDP1C    CD2O1C   CD31C    CD33A        0.1205  3     0.00 !
HDP1C    CD2O1C   CD31C    CD33A        0.0017  6     0.00 !
!allose
OD2C1C   CD2O1C   CD31G    CD31G        0.0012  1   180.00 !
OD2C1C   CD2O1C   CD31G    CD31G        0.1111  2   180.00 !
OD2C1C   CD2O1C   CD31G    CD31G        0.2372  3     0.00 !
OD2C1C   CD2O1C   CD31G    CD31G        0.2931  6   180.00 !
OD2C1C   CD2O1C   CD31G    OD31E        0.3563  1   180.00 !
OD2C1C   CD2O1C   CD31G    OD31E        0.3963  2   180.00 !
OD2C1C   CD2O1C   CD31G    OD31E        0.3065  3   180.00 !
OD2C1C   CD2O1C   CD31G    OD31E        0.0015  6     0.00 !
HDP1C    CD2O1C   CD31G    CD31G        0.0083  1   180.00 !
HDP1C    CD2O1C   CD31G    CD31G        0.0849  2   180.00 !
HDP1C    CD2O1C   CD31G    CD31G        0.2089  3   180.00 !
HDP1C    CD2O1C   CD31G    CD31G        0.2669  6   180.00 !
HDP1C    CD2O1C   CD31G    OD31E        0.3506  1     0.00 !
HDP1C    CD2O1C   CD31G    OD31E        0.4009  2   180.00 !
HDP1C    CD2O1C   CD31G    OD31E        0.3351  3     0.00 !
HDP1C    CD2O1C   CD31G    OD31E        0.0209  6     0.00 !
OD2C1C   CD2O1C   CD31G    HDA1A        0.8416  1     0.00 !
OD2C1C   CD2O1C   CD31G    HDA1A        0.4707  2     0.00 !
OD2C1C   CD2O1C   CD31G    HDA1A        0.1441  3     0.00 !
OD2C1C   CD2O1C   CD31G    HDA1A        0.2459  6     0.00 !
HDP1C    CD2O1C   CD31G    HDA1A        0.8210  1   180.00 !
HDP1C    CD2O1C   CD31G    HDA1A        0.4598  2     0.00 !
HDP1C    CD2O1C   CD31G    HDA1A        0.1146  3   180.00 !
HDP1C    CD2O1C   CD31G    HDA1A        0.2732  6     0.00 !
CD2O1C   CD31G    OD31E    HDP1A        0.2498  1   180.00 !
CD2O1C   CD31G    OD31E    HDP1A        1.3598  2   180.00 !
CD2O1C   CD31G    OD31E    HDP1A        0.0193  3   180.00 !
CD2O1C   CD31G    OD31E    HDP1A        0.1968  6     0.00 !
!psicose
CD31G    CD2O1D   CD32F    OD31E        0.4641  1     0.00 !
CD31G    CD2O1D   CD32F    OD31E        0.4326  2   180.00 !
CD31G    CD2O1D   CD32F    OD31E        0.1294  3     0.00 !
CD31G    CD2O1D   CD32F    OD31E        0.0860  6   180.00 !
OD2C1D   CD2O1D   CD32F    OD31E        0.3933  1   180.00 !
OD2C1D   CD2O1D   CD32F    OD31E        0.6869  2   180.00 !
OD2C1D   CD2O1D   CD32F    OD31E        0.1268  3   180.00 !
OD2C1D   CD2O1D   CD32F    OD31E        0.0412  6     0.00 !
CD31G    CD2O1D   CD32F    HDA2A        0.4743  1   180.00 !
CD31G    CD2O1D   CD32F    HDA2A        0.4251  2     0.00 !
CD31G    CD2O1D   CD32F    HDA2A        0.1273  3     0.00 !
CD31G    CD2O1D   CD32F    HDA2A        0.0222  6   180.00 !
OD2C1D   CD2O1D   CD32F    HDA2A        0.4009  1     0.00 !
OD2C1D   CD2O1D   CD32F    HDA2A        0.6630  2     0.00 !
```

```
OD2C1D   CD2O1D   CD32F    HDA2A        0.1203  3   180.00 !
OD2C1D   CD2O1D   CD32F    HDA2A        0.0433  6     0.00 !
CD32F    CD2O1D   CD31G    CD31G        0.7131  1   180.00 !
CD32F    CD2O1D   CD31G    CD31G        0.0285  2     0.00 !
CD32F    CD2O1D   CD31G    CD31G        0.0334  3   180.00 !
CD32F    CD2O1D   CD31G    CD31G        0.0975  6     0.00 !
OD2C1D   CD2O1D   CD31G    CD31G        0.8248  1     0.00 !
OD2C1D   CD2O1D   CD31G    CD31G        0.1086  2   180.00 !
OD2C1D   CD2O1D   CD31G    CD31G        0.0384  3   180.00 !
OD2C1D   CD2O1D   CD31G    CD31G        0.0570  6   180.00 !
CD32F    CD2O1D   CD31G    HDA1A        0.2186  1   180.00 !
CD32F    CD2O1D   CD31G    HDA1A        0.6386  2     0.00 !
CD32F    CD2O1D   CD31G    HDA1A        0.0179  3     0.00 !
CD32F    CD2O1D   CD31G    HDA1A        0.0144  6     0.00 !
OD2C1D   CD2O1D   CD31G    HDA1A        0.1422  1     0.00 !
OD2C1D   CD2O1D   CD31G    HDA1A        0.8277  2     0.00 !
OD2C1D   CD2O1D   CD31G    HDA1A        0.0736  3   180.00 !
OD2C1D   CD2O1D   CD31G    HDA1A        0.1325  6   180.00 !
CD32F    CD2O1D   CD31G    OD31E        0.9903  1     0.00 !
CD32F    CD2O1D   CD31G    OD31E        0.9450  2   180.00 !
CD32F    CD2O1D   CD31G    OD31E        0.2364  3     0.00 !
CD32F    CD2O1D   CD31G    OD31E        0.0482  6     0.00 !
OD2C1D   CD2O1D   CD31G    OD31E        1.0531  1   180.00 !
OD2C1D   CD2O1D   CD31G    OD31E        1.0554  2   180.00 !
OD2C1D   CD2O1D   CD31G    OD31E        0.2935  3   180.00 !
OD2C1D   CD2O1D   CD31G    OD31E        0.0441  6     0.00 !

IMPROPERS
CD2O1D   CD33C    CD33C    OD2C1D      98.000   0     0.00 !
CD2O1D   CD33C    CD32C    OD2C1D      93.000   0     0.00 !
CD2O1D   CD32C    CD32C    OD2C1D      95.000   0     0.00 !
CD2O1C   HDP1C    CD33C    OD2C1D      75.000   0     0.00 !
CD2O1C   HDP1C    CD32C    OD2C1D      71.300   0     0.00 !
CD2O1C   HDP1C    CD33C    OD2C1C      75.000   0     0.00 !
CD2O1C   HDP1C    CD32C    OD2C1C      71.300   0     0.00 !
CD2O1C   HDP1C    CD31C    OD2C1C      71.300   0     0.00 !
CD2O1C   HDP1C    CD31G    OD2C1C      71.300   0     0.00 !
CD2O1D   CD32F    CD31G    OD2C1D      93.000   0     0.00 !

NONBONDED nbxmod  5 atom vatom cdiel vdistance switch vswitch -
cutnb 16.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

! atom (ignore)   eps       rmin/2
OD2C1C   0.0      -0.175    1.875 ! aldehydes
CD2O1C   0.0      -0.115    1.680 ! aldehydes
OD2C1D   0.0      -0.200    1.85 ! ketones/aldehydes
CD2O1D   0.0      -0.135    1.75 ! ketones
HDP1C    0.0      -0.065    0.95 ! aldehydes

NBFIX
ODW     OD2C1C -0.192     3.61  !Original -0.1921329455 3.66193
ODW     CD2O1C -0.235     3.58  !Original -0.1557513202 3.46692899
ODW     OD2C1D -0.285399  3.63693  !Original -0.2053987585  3.63693
ODW     CD2O1D -0.228752  3.53693  !Original -0.1687523     3.53693
END
```