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Supporting Information for

Multi-Configuration Molecular Mechanics Based on Combined Quantum Mechanical and Molecular Mechanical Calculations

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Table S1. Force Field Parameters for the Reaction OH with Camphor (R2) in the TINKER Parameter File Format for the QM/MM calculation [a]

```
      ##############################
      ##                          ##
      ##  Force Field Definition  ##
      ##                          ##
      ##############################


forcefield              camphor

################################################################################
#  Parameters used for camphor
#
#  This paramter file is specifically generated for H-abstract reaction
#  OH + camphor
#
#  The parameters are mainly taken from charmm27t35.prm, which is the
#  corrected charm27.prm for tinker3.5mn4, with modification as follows:
#
#  (1) Atom type CT0 is all the same as atom type CT1,
#      except that it does not connect to a hydrogen
#      and its charge is set to 0.0.
#
#  (2) Atom type OC is defined as the carboxyl oxygen in tinker 3.5,
#      which is equlivalent to atom type O in original charmm27.
#
#  (3) Atom type CT*, the radical C, is designed as the same as CT2,
#      except that
#       a. the charge is set to -0.09
#       b. the X-CT*-Y angle is set to 120.00, and
#       c. the improper CT*-X-Y-Z  set to   45.0000         0      0.0000
#          (where the force constant is taken from CC-O-CT2-CT1.)
#
#  (4) The tinker 3.5 implementation of the charmm force field is not
#      complete.
#      For the current simultation, missing parameters are taken from the
#      original charmm27 package.
#
#  (5) In order to keep the whole system neutral in charge, the atomic
#      charges for atom types CC, OC, OH1, and H are changed as follows:
#
#      The charges for atom types OC and CC are set to OPLSAA charges, and
#      the charges for atom types OH1 and H are obtained as the ESP charges
#      from model calculations (at the mpwb1k/didz level) on OH radical.
#
################################################################################

vdwtype                 LENNARD-JONES
radiusrule              ARITHMETIC
radiustype              R-MIN
radiussize              RADIUS
```

```
epsilonrule             GEOMETRIC
vdw-14-scale            1.0
chg-14-scale            1.0
dielectric              1.0


      ##############################
      ##                          ##
      ##  Atom Type Definitions   ##
      ##                          ##
      ##############################

atom       1    HA      "Nonpolar Hydrogen"         1      1.008     1
atom       8    H       "Hydroxyl Hydrogen"         1      1.008     1
atom      25    CT1     "Methine Carbon"            6     12.011     4
atom      26    CT2     "Methylene Carbon"          6     12.011     4
atom      27    CT3     "Methyl Carbon"             6     12.011     4
atom      55    CC      "ASP/GLU Carboxylate"       6     12.011     3
atom      76    OH1     "Hydroxyl Oxygen"           8     15.999     2
atom      78    OC      "ASP/GLU Carboxylate"       8     15.999     1
atom      88    HT      "TIP3P Hydrogen"            1      1.008     1
atom     101    OT      "TIP3P Water Oxygen"        8     15.999     2
atom     198    CT*     "C radical"                 6     12.011     3
atom     199    CT0     "sp3 Carbon, no H"          6     12.011     4


      ################################
      ##                            ##
      ##  Van der Waals Parameters  ##
      ##                            ##
      ################################

vdw          1              1.3200    -0.0220
vdw          8              0.2245    -0.0460
vdw         25              2.2750    -0.0200
vdw         26              2.1750    -0.0550
vdw         27              2.0600    -0.0800
vdw         55              2.0000    -0.0700
vdw         76              1.7700    -0.1521
vdw         78              1.7000    -0.1200
vdw         88              0.2245    -0.0460
vdw        101              1.7682    -0.1521
vdw        198              2.2750    -0.0200
vdw        199              2.2750    -0.0200


      ###################################
      ##                               ##
      ##  1-4 Van der Waals Parameters ##
      ##                               ##
      ###################################

vdw14       25              1.9000    -0.0100
vdw14       26              1.9000    -0.0100
vdw14       27              1.9000    -0.0100
vdw14      198              1.9000    -0.0100
vdw14      199              1.9000    -0.0100
```

```
      ###################################
      ##                                 ##
      ##  Bond Stretching Parameters     ##
      ##                                 ##
      ###################################

bond         1   25         309.00     1.1110
bond         1   26         309.00     1.1110
bond         1   27         322.00     1.1110
bond        25   25         222.50     1.5000
bond        25   26         222.50     1.5380
bond        25   27         222.50     1.5380
bond        25   55         200.00     1.5220
bond        26   26         222.50     1.5300
bond        26   27         222.50     1.5280
bond        26   55         200.00     1.5220
bond        27   27         222.50     1.5300
bond        27   55         200.00     1.5220
bond        88  101         450.00     0.9572

bond        26  199         222.50     1.5380
bond        27  199         222.50     1.5380
bond        55  199         200.00     1.5220
bond       199  199         222.50     1.5000

bond        55   78         525.00     1.2600
bond         8   76         545.00     0.9600

bond        25  199         200.00     1.5220

bond         1  198         309.00     1.1110
bond        25  198         222.50     1.5380
bond        26  198         222.50     1.5300
bond        55  198         200.00     1.5220


      ###################################
      ##                                 ##
      ##  Angle Bending Parameters       ##
      ##                                 ##
      ###################################

angle        1   25    1     35.50   109.0000
angle        1   25   25     34.50   110.1000
angle        1   25   26     34.50   110.1000
angle        1   25   27     34.50   110.1000
angle        1   26    1     35.50   109.0000
angle        1   26   25     33.43   110.1000
angle        1   26   26     26.50   110.1000
angle        1   26   27     34.60   110.1000
angle        1   26   55     33.00   109.5000
angle        1   27    1     35.50   108.4000
angle        1   27   25     33.43   110.1000
angle        1   27   26     34.60   110.1000
angle        1   27   27     37.50   110.1000
angle        1   27   55     33.00   109.5000
```

```
angle       25   25   25     53.35   111.0000
angle       25   25   26     53.35   111.0000
angle       25   25   27     53.35   108.5000
angle       26   25   27     53.35   114.0000
angle       27   25   27     53.35   114.0000
angle       25   25   55     52.00   108.0000
angle       55   26   25     52.00   108.0000

angle       25   26   26     58.35   113.5000
angle       55   25   26     52.00   108.0000
angle       55   25   27     52.00   108.0000
angle       25   55   78     40.00   118.0000
angle       26   55   78     40.00   118.0000

angle       25   55   26     40.00   118.00
angle       26   25   26     53.35   112.00

angle        1  199    1     35.50   109.0000
angle        1  199  199     34.50   110.1000
angle        1  199   26     34.50   110.1000
angle        1  199   27     34.50   110.1000
angle        1   26  199     33.43   110.1000
angle        1   27  199     33.43   110.1000
angle      199  199  199     53.35   111.0000
angle      199  199   26     53.35   111.0000
angle      199  199   27     53.35   108.5000
angle       26  199   27     53.35   114.0000
angle       27  199   27     53.35   114.0000
angle      199  199   55     52.00   108.0000
angle       55   26  199     52.00   108.0000
angle      199   26   26     58.35   113.5000
angle       55  199   26     52.00   108.0000
angle       55  199   27     52.00   108.0000
angle      199   55   78     40.00   118.0000
angle      199   55   26     40.00   118.00
angle       26  199   26     53.35   112.00

angle        1   25  199     34.50   110.1000
angle       26   25  199     53.35   111.0000
angle       25  199   27     53.35   108.5000
angle       25  199  199     53.35   111.0000
angle       27  199  199     53.35   108.5000

angle       88  101   88     55.00   104.5200

angle        1  198   25     33.43   120.0000
angle        1  198   26     26.50   120.0000
angle        1  198   55     33.00   120.0000
angle       25  198   26     58.35   120.0000
angle       25  198   55     52.00   120.0000

angle        1   25  198     34.50   110.1000
angle        1   26  198     26.50   110.1000
angle      198   25  199     53.35   111.0000
angle      198   26  199     58.35   113.5000
angle       26   25  198     53.35   112.00
```

```
angle      198   55  199     40.00   118.00
angle      198   55   78     40.00   118.0000


      ################################
      ##                            ##
      ##  Urey-Bradley Parameters   ##
      ##                            ##
      ################################

ureybrad     1   25    1      5.40     1.8020
ureybrad     1   25   25     22.53     2.1790
ureybrad     1   25   26     22.53     2.1790
ureybrad     1   25   27     22.53     2.1790
ureybrad     1   26    1      5.40     1.8020
ureybrad     1   26   25     22.53     2.1790
ureybrad     1   26   26     22.53     2.1790
ureybrad     1   26   27     22.53     2.1790
ureybrad     1   27    1      5.40     1.8020
ureybrad     1   27   25     22.53     2.1790
ureybrad     1   27   26     22.53     2.1790
ureybrad     1   27   27     22.53     2.1790
ureybrad     1   27   55     30.00     2.1630

ureybrad    25   25   25      8.00     2.5610
ureybrad    25   25   26      8.00     2.5610
ureybrad    25   25   27      8.00     2.5610
ureybrad    26   25   27      8.00     2.5610
ureybrad    27   25   27      8.00     2.5610

ureybrad    25   26   26     11.16     2.5610
ureybrad    25   55   78     50.00     2.3880
ureybrad    26   55   78     50.00     2.3880

ureybrad    26   25   26      8.00     2.5610

ureybrad     1  199    1      5.40     1.8020
ureybrad     1  199  199     22.53     2.1790
ureybrad     1  199   26     22.53     2.1790
ureybrad     1  199   27     22.53     2.1790
ureybrad     1   26  199     22.53     2.1790
ureybrad     1   27  199     22.53     2.1790
ureybrad   199  199  199      8.00     2.5610
ureybrad   199  199   26      8.00     2.5610
ureybrad   199  199   27      8.00     2.5610
ureybrad    26  199   27      8.00     2.5610
ureybrad    27  199   27      8.00     2.5610
ureybrad   199   26   26     11.16     2.5610
ureybrad   199   55   78     50.00     2.3880
ureybrad    26  199   26      8.00     2.5610

ureybrad     1   25  199     22.53     2.1790
ureybrad    26   25  199      8.00     2.5610
ureybrad    25  199   27      8.00     2.5610
ureybrad    25  199  199      8.00     2.5610
ureybrad    27  199  199      8.00     2.5610
```

```
ureybrad     1  198   25      22.53     2.1790
ureybrad     1  198   26      22.53     2.1790
ureybrad    25  198   26      11.16     2.5610
ureybrad     1   25  198      22.53     2.1790
ureybrad     1   26  198      22.53     2.1790
ureybrad   198   25  199       8.00     2.5610
ureybrad   198   26  199      11.16     2.5610
ureybrad    26   25  198       8.00     2.5610
ureybrad   198   55   78      50.00     2.3880


      ############################
      ##                        ##
      ##  Torsional Parameters  ##
      ##                        ##
      ############################

torsion     78   55   26    1          0.050  180.0  6
torsion     78   55   26   25          0.050  180.0  6
torsion     78   55   26  199          0.050  180.0  6
torsion      1   25   26    1          0.200    0.0  3
torsion      1  199   26    1          0.200    0.0  3

torsion     55   26   25   78         45.000    0.0  0
torsion     55   26  199   78         45.000    0.0  0

#charmm27    X  CT1   CC    X        0.0500  6   180.00
torsion      1   25   55    1          0.050  180.0  6
torsion      1  199   55    1          0.050  180.0  6
torsion    199  199   55   78          0.050  180.0  6
torsion     26  199   55   78          0.050  180.0  6
torsion    199  199   55   26          0.050  180.0  6
torsion     26  199   55   26          0.050  180.0  6
torsion     27  199   55   26          0.050  180.0  6
torsion     27  199   55   78          0.050  180.0  6

#charmm27   X    CT2  CC   X        0.0500  6   180.00 ! ALLOW   POL PEP
torsion      1   26   55  199          0.050  180.0  6
torsion     25   26   55  199          0.050  180.0  6

#charmm27   X    CT1  CT1  X        0.2000  3     0.00 ! ALLOW   ALI
torsion      1   25   25    1          0.200    0.0  3
torsion      1   25  199   27          0.200    0.0  3
torsion      1   25  199  199          0.200    0.0  3
torsion     26   25  199   27          0.200    0.0  3
torsion     26   25  199  199          0.200    0.0  3
torsion     25  199  199   26          0.200    0.0  3
torsion     25  199  199   27          0.200    0.0  3
torsion     25  199  199   55          0.200    0.0  3
torsion     26  199  199   27          0.200    0.0  3
torsion     27  199  199   27          0.200    0.0  3
torsion     27  199  199   55          0.200    0.0  3
torsion    198   25  199  199          0.200    0.0  3
torsion    198   25  199   27          0.200    0.0  3

#charmm27   X    CT1  CT2  X        0.2000  3     0.00 ! ALLOW   ALI
torsion      1   25   26    1          0.200    0.0  3
```

```
torsion      1   25   26   26           0.200     0.0  3
torsion      1   25   26   55           0.200     0.0  3
torsion     26   25   26   26           0.200     0.0  3
torsion     26   25   26   55           0.200     0.0  3
torsion    199   25   26    1           0.200     0.0  3
torsion    199   25   26   26           0.200     0.0  3
torsion    199   25   26   55           0.200     0.0  3
torsion      1   26   25   26           0.200     0.0  3
torsion      1   26  199    1           0.200     0.0  3
torsion      1   26  199   27           0.200     0.0  3
torsion      1   26  199   55           0.200     0.0  3
torsion      1   26  199  199           0.200     0.0  3
torsion     26   26  199   27           0.200     0.0  3
torsion     26   26  199   55           0.200     0.0  3
torsion     26   26  199  199           0.200     0.0  3
torsion    198   25   26   55           0.200     0.0  3
torsion      1   26   25  198           0.200     0.0  3
torsion    198   26  199   55           0.200     0.0  3
torsion    198   26  199  199           0.200     0.0  3
torsion    198   26  199   27           0.200     0.0  3
torsion      1  198   25   26           0.200     0.0  3
torsion     26   25  198   26           0.200     0.0  3
torsion      1   25  198    1           0.200     0.0  3
torsion    199   25  198    1           0.200     0.0  3
torsion      1   25  198   26           0.200     0.0  3
torsion    199   25  198   26           0.200     0.0  3

#charmm27  X    CT2  CT2  X        0.1950  3     0.00 ! ALLOW   ALI
torsion      1   26   26    1           0.195     0.0  3
torsion      1   26   26   25           0.195     0.0  3
torsion      1   26   26  199           0.195     0.0  3
torsion     25   26   26  199           0.195     0.0  3
torsion      1  198   26  199           0.195     0.0  3
torsion      1   26  198   25           0.195     0.0  3
torsion      1  198   26    1           0.195     0.0  3
torsion     25  198   26  199           0.195     0.0  3

#charmm27  X    CT1  CT3  X        0.2000  3     0.00 ! ALLOW   ALI
torsion      1   25   27    1           0.200     0.0  3
torsion      1   27  199    1           0.200     0.0  3
torsion      1   27  199   25           0.200     0.0  3
torsion      1   27  199   26           0.200     0.0  3
torsion      1   27  199   27           0.200     0.0  3
torsion      1   27  199   55           0.200     0.0  3
torsion      1   27  199  199           0.200     0.0  3


      ####################################
      ##                                ##
      ##  Improper Dihedral Parameters  ##
      ##                                ##
      ####################################

#charmm27    CC   CT2  CT1  O   45.0000         0      0.0000
improper     55   26   25   78         45.000   0.0  0
improper     55   26  199   78         45.000   0.0  0
```

```
#hailin    CT*  CT1  CT2   H   45.0000          0       0.0000
improper    198   25   26    1          45.000    0.0   0


      ########################################
      ##                                    ##
      ##  Atomic Partial Charge Parameters  ##
      ##                                    ##
      ########################################

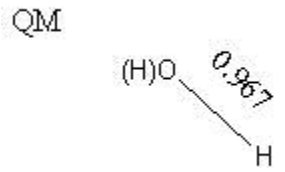
charge       1          0.090
charge       8          0.404
charge      25         -0.090
charge      26         -0.180
charge      27         -0.270
charge      55          0.470
charge      76         -0.404
charge      78         -0.470
charge      88          0.417
charge     101         -0.834
charge     198         -0.090
charge     199          0.000
```

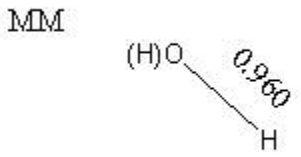
[a] Distance in Å, angle in degree, and charge in electron. See the web page of TINKER (http://dasher.wustl.edu/tinker/) and MC-TINKER (http://comp.chem.umn.edu/mc-tinker/) for details about the format of the parameter file. The MC-TINKER version 1.1 is based on the TINKER3.5MN3, which is locally modified version of TINKER3.5.

Table S2. Comparison of Selected Geometric Data Optimized at the QM, the MM, and the QM/MM level for the Reactant and Product in the Reaction OH with Camphor (R2). [a]

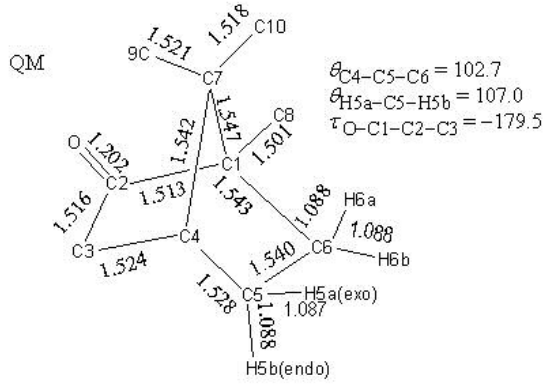
Reactant:

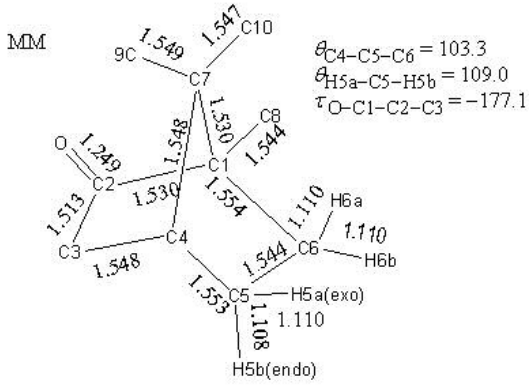
OH

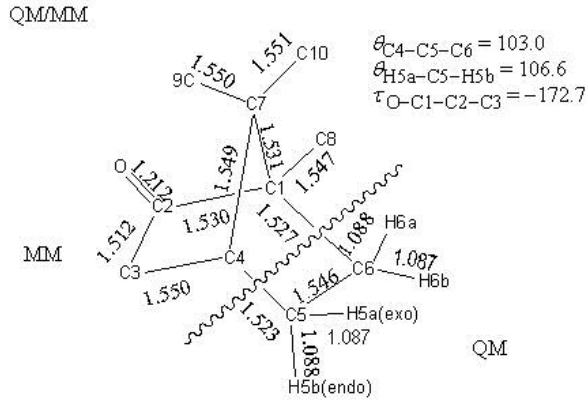




Camphor



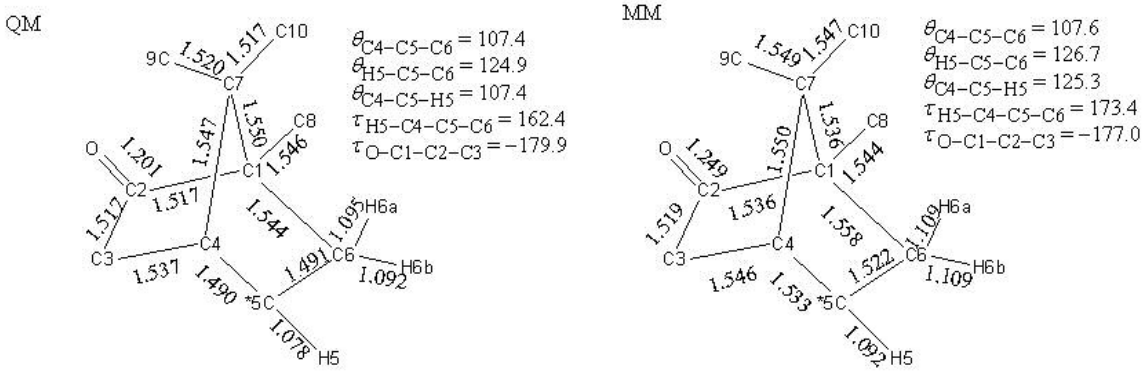


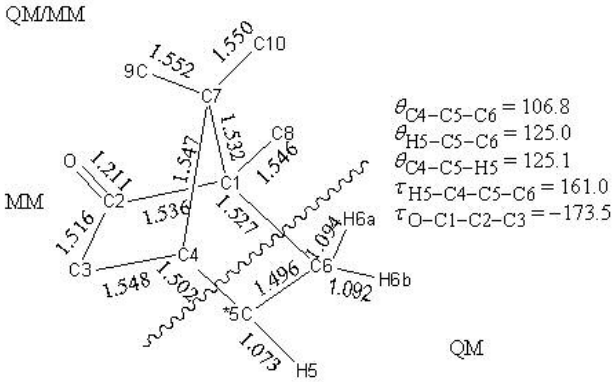


Product:

H_2O

Camphor Radical

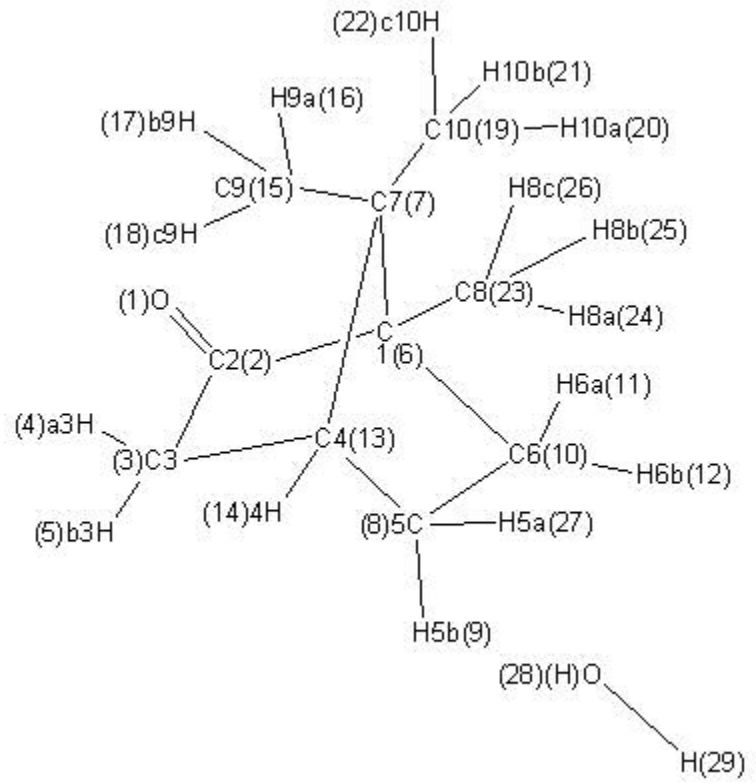




[c] The MPWB1K/DIDZ level of theory in QM calculations, and CHARMM27 force field for MM calculations. See Table S1 in supporting information for MM parameters. See Figure 2 for the QM/MM boundary setup. The electrostatic

embedding (EE) scheme redistributed charge and dipole (RCD) was used in QM/MM computations. Distance is in Å, and angles in degree. OW and HW denote the oxygen and hydrogen atoms in a water molecule, and C5* denotes the carbon radical in the product.

Table S3. The redundant internal coordinated used for generalized normal mode analysis the Reaction OH with Camphor (R2). [a]



1-2	2-3	2-6	3-4	3-5
3-13	6-7	6-10	6-23	7-13
7-15	7-19	8-9	8-10	8-13
8-27	10-11	10-12	13-14	15-16
15-17	15-18	19-20	19-21	19-22
23-24	23-25	23-26		
28-29				

1-2-3	1-2-6	3-2-6		
2-3-4	2-3-5	2-3-13	4-3-5	4-3-13
2-6-7	2-6-10	2-6-23	7-6-10	7-6-23
6-7-13	6-7-15	6-7-19	13-7-15	13-7-19
9-8-10	9-8-13	9-8-27	10-8-13	10-8-27
6-10-8	6-10-11	6-10-12	8-10-11	8-10-12
3-13-7	3-13-8	3-13-14	7-13-8	7-13-14
7-15-16	7-15-17	7-15-18	16-15-17	16-15-18
7-19-20	7-19-21	7-19-22	20-19-21	20-19-22
6-23-24	6-23-25	6-23-26	24-23-25	24-23-26

3-1-2-6				
1-2-3-4	1-2-3-5	1-2-3-13	6-2-3-4	6-2-3-5
1-2-6-7	1-2-6-10	1-2-6-23	3-2-6-7	3-2-6-10
2-3-13-7	2-3-13-8	2-3-13-14	4-3-13-7	4-3-13-8
2-6-7-13	2-6-7-15	2-6-7-19	10-6-7-13	10-6-7-15
2-6-10-8	2-6-10-11	2-6-10-12	7-6-10-8	7-6-10-11
2-6-23-24	2-6-23-25	2-6-23-26	7-6-23-24	7-6-23-25
6-7-13-3	6-7-13-8	6-7-13-14	15-7-13-3	15-7-13-8

6-7-15-16	6-7-15-17	6-7-15-18	13-7-15-16	13-7-15-17
6-7-19-20	6-7-19-21	6-7-19-22	13-7-19-20	13-7-19-21
9-8-10-6	9-8-10-11	9-8-10-12	13-8-10-6	13-8-10-11
9-8-13-3	9-8-13-7	9-8-13-14	10-8-13-3	10-8-13-7
8-28	9-28	27-28		
9-28-29	27-28-29			
8-9-28	8-27-28			
9-8-28-29	27-8-28-29	10-8-28-29		
10-8-9-28	13-8-9-28	10-8-27-28		
27-8-28-9				

[a] The index for each atom is given in parentheses, A–B indicates a stretch of the A–B bond, A–B–C indicates a bend of the A–B–C angle, and A–B–C–D indicates a torsion of the dihedral A–B–C–D.

Table S4. Vibrational Frequencies of the Generalized Normal Modes at the Reactant, Saddle Point, and Product for the Reaction OH with Propane (R1). [a]

Integral grid	QM Ultrafine	QM Fine			QM/MM Ultrafine		
Ref.	This Work	Lin2004 [b]			This Work		
	ν	ν	Δν	| Δν |	ν	Δν	| Δν |
C3H8	3199	3199	0	0	3206	6	6
	3197	3197	0	0	3200	2	2
	3196	3197	0	0	3180	–17	17
	3187	3188	1	1	3139	–48	48
	3150	3151	1	1	3119	–31	31
	3116	3117	1	1	2968	–147	147
	3112	3113	0	0	2967	–146	146
	3110	3110	0	0	2866	–244	244
	1550	1550	0	0	1551	1	1
	1546	1545	0	0	1546	0	0
	1535	1534	0	0	1513	–22	22
	1530	1530	0	0	1489	–41	41
	1527	1526	0	0	1463	–64	64
	1460	1460	0	0	1457	–2	2
	1451	1451	0	0	1452	1	1
	1400	1400	1	1	1403	3	3
	1348	1348	0	0	1336	–12	12
	1242	1243	0	0	1151	–91	91
	1211	1210	0	0	1141	–69	69
	1109	1109	0	0	1118	9	9
	954	954	0	0	967	13	13
	930	931	1	1	965	34	34

	913	913	0	0	901	−12	12
	767	767	1	1	786	19	19
	375	373	−1	1	383	8	8
	281	278	−3	3	272	−9	9
	226	222	−4	4	223	−2	2
Ave			0	1		−32	39
OH	3890	3890	0	0	3890	0	0
Ave			0	0		0	0
C3H7	3344	3344	1	1	3349	6	6
	3235	3236	1	1	3241	6	6
	3207	3207	0	0	3188	−19	19
	3200	3200	0	0	3132	−68	68
	3158	3159	1	1	2968	−190	190
	3115	3116	0	0	2967	−149	149
	3112	3113	1	1	2865	−247	247
	1545	1545	0	0	1525	−20	20
	1534	1533	0	0	1495	−38	38
	1527	1527	0	0	1458	−69	69
	1506	1506	0	0	1457	−49	49
	1439	1440	0	0	1443	4	4
	1367	1368	1	1	1378	11	11
	1341	1342	1	1	1326	−15	15
	1226	1226	0	0	1149	−77	77
	1133	1134	0	0	1131	−3	3
	1076	1077	0	0	1031	−45	45
	934	934	0	0	957	23	23
	915	915	1	1	931	17	17
	763	763	0	0	783	20	20

	541	541	1	1	549	9	9
	344	344	0	0	357	13	13
	259	256	−3	3	234	−25	25
	45	35	−10	10	114	70	70
Ave			0	1		−35	50
H2O	4119	4115	−5	5	4119	0	0
	3992	3988	−5	5	3992	0	0
	1647	1647	1	1	1647	0	0
Ave			−3	3		0	0
Saddle point	3924	3924	0	0	3923	0	0
	3232	3232	0	0	3242	9	9
	3202	3202	0	0	3203	1	1
	3201	3201	0	0	3163	−38	38
	3173	3173	0	0	3152	−21	21
	3153	3153	0	0	2969	−185	185
	3133	3133	0	0	2967	−166	166
	3115	3115	0	0	2866	−249	249
	1544	1544	0	0	1522	−23	23
	1535	1535	0	0	1511	−24	24
	1530	1530	0	0	1470	−60	60
	1508	1508	0	0	1462	−46	46
	1448	1448	0	0	1457	8	8
	1403	1403	0	0	1407	4	4
	1391	1391	0	0	1397	6	6
	1354	1354	0	0	1355	1	1
	1311	1311	0	0	1306	−6	6
	1234	1234	0	0	1206	−28	28
	1229	1229	0	0	1145	−84	84

	1124	1124	0	0	1132	8	8
	1050	1050	0	0	1030	–20	20
	947	947	0	0	965	17	17
	932	932	0	0	942	10	10
	911	911	0	0	926	15	15
	771	771	0	0	793	22	22
	644	644	0	0	660	16	16
	416	416	0	0	419	3	3
	356	356	0	0	364	8	8
	249	249	0	0	236	–14	14
	107	107	0	0	106	–1	1
	82	82	0	0	84	2	2
	22	15	–7	7	22	0	0
	–1004	–1005	–1	1	–958	46	46
Ave			0	0		–24	35

[a] In the previous paper (see footnote b), the DFT Integral was performed by use of the option of (Grid=Fine) in the calculations of vibrational frequencies by *Gaussian03*. In this work, the option of (Grid=Ultrafine) is used. Frequency in cm^{-1}.

[b] Lin, H.; Pu, J. Z.; Albu, T. V.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 4112.

Table S5. Vibrational Frequencies of the Generalized Normal Modes at the Reactant, Saddle Point, and Product for the Reaction OH with Camphor (R2). [a]

Reactant			Product		
QM	QM/MM	QM/MM – QM	QM	QM/MM	QM/MM – QM
3865	3865	0	3297	3385	87
3220	3240	20	3214	3169	-44
3208	3219	11	3209	3119	-90
3206	3189	-17	3204	2950	-254
3201	3178	-24	3204	2934	-270
3200	2947	-252	3198	2933	-266
3196	2934	-262	3192	2931	-262
3192	2933	-260	3187	2930	-257
3187	2932	-255	3184	2928	-255
3182	2930	-252	3143	2927	-215
3176	2929	-247	3123	2881	-242
3149	2928	-221	3120	2880	-240
3148	2881	-267	3115	2880	-235
3138	2880	-258	3112	2879	-234
3118	2880	-239	3073	2841	-232
3117	2879	-238	1916	1543	-373
3113	2840	-273	1546	1531	-15
1915	1583	-332	1543	1522	-21
1559	1559	0	1526	1504	-22
1547	1529	-18	1522	1462	-60
1543	1521	-22	1517	1455	-62
1531	1505	-26	1511	1453	-58
1524	1461	-63	1499	1447	-52

1519	1457	-62	1481	1444	-37
1513	1453	-60	1453	1428	-25
1508	1447	-61	1445	1426	-19
1484	1446	-39	1435	1418	-17
1454	1428	-27	1395	1372	-23
1446	1425	-20	1374	1364	-10
1437	1416	-21	1359	1336	-23
1400	1370	-31	1330	1324	-6
1373	1355	-18	1316	1294	-22
1362	1343	-19	1290	1270	-20
1350	1339	-11	1252	1247	-5
1321	1316	-4	1242	1203	-39
1308	1299	-9	1229	1187	-42
1287	1273	-15	1193	1184	-9
1255	1252	-3	1186	1132	-54
1254	1210	-44	1132	1108	-24
1222	1193	-29	1106	1077	-30
1218	1186	-32	1090	1042	-48
1191	1157	-35	1056	1024	-33
1140	1118	-22	1033	1017	-16
1124	1083	-41	1010	999	-10
1103	1047	-56	995	982	-13
1071	1023	-48	987	962	-25
1054	1013	-41	977	957	-20
1029	1000	-29	956	939	-17
1000	990	-10	939	925	-14
986	972	-15	919	900	-19
980	957	-23	889	869	-20
963	950	-13	799	796	-4
952	922	-30	740	700	-41
909	894	-15	677	606	-71

895	871	-23	631	550	-81
861	853	-8	604	539	-65
789	794	5	586	512	-75
739	692	-47	535	484	-50
676	602	-73	488	470	-18
629	542	-87	458	453	-5
590	531	-59	394	402	8
565	498	-66	388	397	9
534	469	-65	319	362	44
483	456	-27	314	336	22
421	420	0	277	300	23
399	402	3	264	282	18
389	384	-5	244	264	20
312	335	22	228	257	30
301	314	13	223	232	10
264	282	18	188	227	39
246	265	19	177	210	33
230	257	27	110	117	7
226	234	8			
183	227	43			
165	207	41			
105	118	13			

Saddle Point

H5a(exo)			H5b(endo)		
QM	QM/MM	QM/MM – QM	QM	QM/MM	QM/MM – QM
3902	3917	15	3902	3906	4
3237	3240	3	3216	3246	29

3209	3227	17	3213	3231	17
3205	3183	-22	3209	3186	-24
3205	2949	-256	3204	2949	-256
3198	2934	-264	3202	2934	-269
3196	2934	-262	3193	2933	-261
3191	2933	-258	3192	2931	-260
3190	2930	-260	3189	2930	-259
3186	2929	-257	3186	2929	-257
3173	2927	-245	3178	2927	-250
3150	2883	-267	3156	2881	-275
3136	2880	-255	3137	2880	-257
3121	2880	-241	3119	2880	-239
3120	2879	-241	3117	2879	-238
3115	2841	-274	3114	2842	-273
1917	1565	-352	1919	1559	-360
1556	1532	-24	1548	1534	-13
1547	1526	-21	1544	1525	-19
1540	1516	-24	1530	1511	-19
1530	1507	-24	1528	1461	-67
1522	1463	-60	1519	1456	-62
1518	1459	-59	1514	1453	-61
1513	1453	-60	1508	1447	-61
1506	1448	-58	1490	1445	-45
1482	1447	-36	1455	1428	-27
1459	1428	-31	1446	1425	-21
1447	1425	-22	1444	1418	-26
1442	1418	-24	1434	1392	-43
1399	1369	-30	1399	1368	-31
1370	1356	-14	1365	1350	-15
1354	1344	-10	1357	1349	-8
1333	1335	2	1346	1341	-4

1314	1302	-12	1320	1307	-13
1299	1275	-25	1299	1304	4
1276	1258	-18	1262	1269	7
1254	1231	-23	1252	1253	1
1233	1201	-32	1243	1219	-23
1224	1190	-34	1240	1193	-46
1192	1182	-10	1195	1191	-4
1186	1138	-48	1186	1162	-25
1176	1113	-62	1178	1136	-41
1141	1085	-56	1134	1093	-41
1122	1062	-60	1120	1059	-61
1084	1037	-47	1094	1032	-62
1071	1017	-55	1064	1025	-39
1053	1009	-44	1055	1011	-44
1032	997	-35	1033	999	-33
999	991	-8	1007	972	-35
995	973	-22	986	959	-27
988	958	-29	980	953	-27
981	956	-25	968	931	-37
953	929	-25	952	913	-39
923	913	-10	929	896	-33
897	881	-17	897	869	-28
889	870	-18	874	851	-23
801	796	-5	789	793	3
738	700	-38	755	705	-50
695	640	-55	696	663	-33
674	578	-95	649	591	-58
627	539	-88	632	547	-84
588	530	-58	588	530	-58
536	485	-50	554	491	-62
532	459	-73	531	468	-63

484	456	-28	481	456	-25
418	415	-3	418	414	-4
400	406	6	392	399	7
392	381	-11	389	378	-11
324	354	30	316	341	25
302	320	18	291	297	6
270	286	15	266	283	17
247	267	19	244	264	20
234	259	25	230	256	26
230	249	19	226	232	7
198	226	28	185	226	41
181	224	43	170	212	43
127	130	3	120	134	14
122	96	-26	84	101	17
84	80	-4	76	66	-10
61	44	-17	60	64	4

[a] The option of (Grid=Ultrafine) is used. Frequency in cm^{-1}. The mean signed error (MSE) of the QM/MM frequencies in comparison with the QM frequencies is –61, –62, –62, and –61 cm^{-1} for the reactant, the product, the saddle point of H5a(exo), and the saddle point of H5b(endo), respectively. The mean unsigned error (MUE) is 67, 72, 71, and 71cm^{-1}, respectively.

Table S6. Force Field Parameters for the Reaction OH with Camphor (R2) in the TINKER Parameter File Format for the MC-TINKERATE calculation [a]

```
      ##############################
      ##                          ##
      ##  Force Field Definition  ##
      ##                          ##
      ##############################


forcefield              MM3-1996

bondunit                71.94
bond-cubic              -2.55
bond-quartic            3.793125        !! (7/12) * bond-cubic^2
angleunit               0.02191418
angle-cubic             -0.014
angle-quartic           0.000056
angle-pentic            -0.0000007
angle-sextic            0.000000022
strbndunit              2.51118
angangunit              -0.02191418
torsionunit             0.5
strtorunit              -5.9975
vdwtype                 BUCKINGHAM
radiusrule              ARITHMETIC
radiustype              R-MIN
radiussize              RADIUS
epsrule                 GEOMETRIC
vdw-14-scale            1.0
a-expterm               184000.0
b-expterm               12.0
c-expterm               2.25
chg-14-scale            1.0
dielectric              1.5


      ##############################
      ##                          ##
      ##  Literature References  ##
      ##                          ##
      ##############################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```

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11, 868-895, 1990

All parameters in this file are adapted from "MM3(96) Parameter Set",
dated October 15, 1996 as obtained from the Allinger Group's web site
located at http://europa.chem.uga.edu/ccmsd/mm2mm3.html and the MM3
Parameter Search site at http://europa.chem.uga.edu/cgi-bin/mm3para


      ##############################
      ##                          ##
      ##  Atom Type Definitions   ##
      ##                          ##
      ##############################


atom      1    C     "CSP3 ALKANE"              6     12.000     4
atom      2    C     "CSP2 ALKENE"              6     12.000     3
atom      3    C     "CSP2 CARBONYL"            6     12.000     3
atom      4    C     "CSP ALKYNE"               6     12.000     2
atom      5    H     "EXCEPT ON N,O,S"          1      1.008     1
atom      6    O     "C-O-H, C-O-C, O-O"        8     15.995     2
atom      7    O     "O=C CARBONYL"             8     15.995     1
atom     20    *     "NOT USED"                 0      0.000     0
atom     21    H     "-OH ALCOHOL"              1      1.008     1
atom     22    C     "CYCLOPROPANE"             6     12.000     4
atom     23    H     "NH AMINE/IMINE"           1      1.008     1
atom     24    H     "COOH CARBOXYL"            1      1.008     1
atom     28    H     "H-N-C=O AMIDE"            1      1.008     1
atom     29    C*    "RADICAL"                  6     12.000     3


      ################################
      ##                            ##
      ##  Van der Waals Parameters  ##
      ##                            ##
      ################################


vdw          1              2.040      0.027
vdw          2              1.960      0.056
vdw          3              1.940      0.056
vdw          4              1.940      0.056
```

```
vdw             5                1.620      0.020      0.923
vdw             6                1.820      0.059
vdw             7                1.820      0.059
vdw             8                1.930      0.043
vdw             9                1.930      0.043
vdw            10                1.930      0.043
vdw            11                1.710      0.075
vdw            12                2.070      0.240
vdw            13                2.220      0.320
vdw            14                2.360      0.424
vdw            15                2.150      0.202
vdw            16                2.150      0.202
vdw            17                2.150      0.202
vdw            18                2.150      0.202
vdw            19                2.290      0.140
vdw            20                0.000      0.000
vdw            21                1.600      0.016      0.923
vdw            22                1.940      0.045
vdw            23                1.600      0.018      0.923
vdw            24                0.900      0.015      0.923
vdw            25                2.220      0.168
vdw            26                2.150      0.014
vdw            27                2.150      0.014
vdw            28                1.600      0.015      0.923
vdw            29                1.940      0.030


      ######################################
      ##                                  ##
      ##  Van der Waals Pair Parameters   ##
      ##                                  ##
      ######################################


vdwpr          1    5           3.560      0.023
vdwpr          1   36           3.557      0.023
vdwpr          2   21           2.650      0.550
vdwpr          2   23           3.000      0.100
vdwpr          2   28           2.620      0.860
vdwpr          2   44           2.830      0.200
vdwpr          2   73           3.000      0.750
vdwpr          2  124           2.960      0.250
vdwpr          4   21           2.600      0.510
vdwpr          4   23           2.870      0.260
vdwpr          4   28           2.540      0.930
vdwpr          4  124           2.820      0.340
vdwpr          6   21           2.110      3.000
vdwpr          6   23           2.380      1.300
vdwpr          6   24           2.140      3.300
vdwpr          6   28           2.030      5.140
vdwpr          6   44           2.680      0.150
vdwpr          6   48           1.880     12.000
vdwpr          6   73           2.250      3.150
vdwpr          6  124           2.300      1.700
vdwpr          7   21           2.070      2.550
vdwpr          7   23           2.390      1.100
vdwpr          7   24           2.050      3.000
```

vdwpr	7	28	2.070	4.440
vdwpr	7	48	2.000	6.000
vdwpr	7	73	2.030	5.100
vdwpr	7	124	2.330	1.390
vdwpr	8	21	2.150	4.700
vdwpr	8	23	2.400	2.280
vdwpr	8	24	2.220	2.100
vdwpr	8	28	2.130	7.780
vdwpr	8	73	2.220	1.500
vdwpr	8	124	2.300	3.530
vdwpr	11	21	2.050	0.450
vdwpr	11	23	2.050	0.300
vdwpr	11	24	2.050	0.900
vdwpr	11	28	2.050	0.600
vdwpr	11	73	2.050	0.600
vdwpr	12	21	2.800	1.100
vdwpr	12	23	3.140	0.440
vdwpr	12	24	2.430	0.900
vdwpr	12	28	2.770	1.820
vdwpr	12	73	2.430	0.600
vdwpr	12	124	3.090	0.670
vdwpr	13	21	2.580	1.200
vdwpr	13	23	2.580	0.300
vdwpr	13	24	2.580	0.900
vdwpr	13	28	2.580	0.600
vdwpr	13	73	2.580	0.600
vdwpr	14	21	2.720	0.900
vdwpr	14	23	2.720	0.600
vdwpr	14	24	2.720	0.600
vdwpr	14	28	2.720	0.300
vdwpr	14	73	2.720	0.300
vdwpr	15	21	2.680	1.350
vdwpr	15	23	2.510	0.300
vdwpr	15	24	2.510	0.600
vdwpr	15	28	2.510	0.300
vdwpr	15	44	2.940	0.700
vdwpr	15	73	2.510	0.300
vdwpr	17	21	2.550	0.600
vdwpr	17	23	2.550	0.150
vdwpr	17	24	2.550	0.300
vdwpr	17	28	2.550	0.300
vdwpr	17	73	2.550	0.300
vdwpr	19	113	2.450	15.000
vdwpr	19	114	2.450	15.000
vdwpr	21	22	2.400	1.060
vdwpr	21	37	1.740	3.720
vdwpr	21	47	2.070	5.000
vdwpr	21	50	2.650	0.550
vdwpr	21	79	1.950	3.460
vdwpr	22	23	2.690	0.427
vdwpr	22	28	2.370	1.756
vdwpr	22	124	2.630	0.658
vdwpr	23	37	2.250	0.675
vdwpr	23	47	2.310	2.430
vdwpr	23	50	3.000	0.100
vdwpr	23	79	2.190	1.590
vdwpr	23	150	2.400	2.280

```
vdwpr         24   37          2.220       2.100
vdwpr         24   75          2.140       1.450
vdwpr         24   77          1.830       4.950
vdwpr         28   37          2.220       1.500
vdwpr         28   47          2.050       8.280
vdwpr         28   50          3.000       0.750
vdwpr         28   79          1.960       5.240


      ###################################
      ##                               ##
      ##  Bond Stretching Parameters   ##
      ##                               ##
      ###################################


bond           1    1         4.4900     1.5247
bond           1    2         6.3000     1.4990
bond           1    3         4.8000     1.5090
bond           1    4         5.5000     1.4700
#bond          1    5         4.7400     1.1120
bond           1    6         5.7000     1.4130
bond           1    8         5.3000     1.4480
bond           1    9         5.2100     1.4460
bond           1   11         5.9000     1.3920
bond           1   12         3.1000     1.7910
bond           1   13         2.3000     1.9440
bond           1   14         2.1500     2.1660
bond           1   15         3.0000     1.8050
bond           1   16         3.2130     1.8160
bond           1   17         2.9500     1.8000
bond           1   18         3.1000     1.7720
bond           1   19         3.0500     1.8760
bond           1   22         5.0000     1.5110
bond           1   25         2.9400     1.8430
bond           1   26         4.5014     1.5769
bond           1   29         5.2000     1.4990
bond           3    3        11.2500     1.2170
bond           3    5         4.3700     1.1180
bond           3    6         6.0000     1.3538
bond           3    7        10.1000     1.2080
bond           3    9         6.7000     1.3770
bond           3   11         4.2000     1.3810
bond           3   12         2.8800     1.8160
bond           3   13         2.8000     1.9900
bond           3   14         2.6000     2.2280
bond           3   22         4.4000     1.4470
bond           5   16         3.8000     1.3460
bond           5   17         3.1700     1.3720
bond           5   18         3.8000     1.3460
bond           5   19         2.6500     1.4830
bond           5   22         5.0800     1.0860
bond           5   25         3.0650     1.4200
bond           5   29         5.2200     1.1010
bond           6    6         3.9500     1.4480
bond           6   19         5.0500     1.6360
#bond          6   21         7.6300     0.9470
```

```
      ##########################################
      ##                                      ##
      ##  Bond Stretching Parameters (5-Ring)  ##
      ##                                      ##
      ##########################################


bond5         1    1         4.4900     1.5258
bond5         1    2         6.3000     1.5120
bond5         1    3         4.8000     1.5140
bond5         1    6         5.7000     1.4160
bond5         1    8         5.3000     1.4530
bond5         1    9         5.2100     1.4700
bond5         1   15         3.0000     1.8080
bond5         1   18         3.1000     1.7800
bond5         1   19         2.8500     1.8840
bond5         1   22         5.0000     1.5100
bond5         1   29         5.2000     1.4990
bond5         2    2         7.7000     1.3340
bond5         2    3         9.6000     1.3510
bond5         2    6         6.0000     1.3550
bond5         2   18         2.8000     1.7720
bond5         2   19         3.0000     1.8560
bond5         3    3         9.6000     1.3340
bond5         3    6         5.8000     1.3550
bond5         3    9         6.8300     1.3770
bond5         6    6         3.9500     1.4550
bond5         6   56         3.0000     1.4180


      ##################################
      ##                              ##
      ##  Angle Bending Parameters    ##
      ##                              ##
      ##################################


angle         1    1    1     0.670    109.500    110.200    111.000
angle         1    1    2     0.540    110.600    109.800    110.600
angle         1    1    3     0.800    110.600    110.600    110.600
angle         1    1    4     0.960    108.800    109.700    110.000
angle         1    1    5     0.590    109.800    109.310    110.700
angle         1    1    6     0.830    107.500    107.000    107.900
angle         1    1    8     0.780    109.470    108.000    111.000
angle         1    1    9     0.750    109.480    111.300    111.800
angle         1    1   11     0.920    110.800    109.500    109.100
angle         1    1   12     0.800    106.200    106.400    108.000
angle         1    1   13     0.740    108.200      0.000      0.000
angle         1    1   14     0.650    106.000    107.200    107.000
angle         1    1   15     0.740    108.000    109.500    110.100
angle         1    1   16     0.420    107.800      0.000      0.000
angle         1    1   17     0.650    107.500    104.700    106.000
angle         1    1   18     0.870    103.000      0.000      0.000
```

angle	1	1	19	0.400	109.000	112.700	111.500
angle	1	1	22	0.350	114.400	112.600	114.400
angle	1	1	25	0.600	107.500	109.600	108.000
angle	1	1	26	0.378	110.920	0.000	0.000
angle	1	1	29	0.450	110.000	0.000	0.000
angle	2	1	2	0.450	113.200	115.500	113.000
angle	2	1	3	0.470	109.470	110.510	110.200
angle	2	1	4	0.570	109.470	110.510	110.200
angle	2	1	5	0.550	109.500	109.310	110.400
angle	2	1	6	0.700	107.000	0.000	0.000
angle	2	1	8	1.045	110.740	0.000	0.000
angle	2	1	9	0.500	109.800	0.000	0.000
angle	2	1	11	0.760	109.000	0.000	0.000
angle	2	1	12	0.650	109.500	0.000	0.000
angle	2	1	14	0.695	109.300	0.000	0.000
angle	2	1	15	0.650	107.800	107.800	113.900
angle	2	1	16	0.420	107.800	0.000	0.000
angle	2	1	19	0.500	109.500	105.000	109.500
angle	2	1	22	0.450	112.400	0.000	0.000
angle	3	1	3	0.470	109.470	110.510	110.200
angle	3	1	5	0.540	109.490	109.490	109.490
angle	3	1	6	0.700	109.500	0.000	0.000
angle	3	1	8	1.045	110.740	0.000	0.000
angle	3	1	9	0.850	109.500	110.600	112.300
angle	3	1	11	0.760	109.200	0.000	0.000
angle	3	1	12	0.650	109.800	0.000	0.000
angle	3	1	13	0.750	109.100	0.000	0.000
angle	3	1	14	0.600	108.900	0.000	0.000
angle	3	1	15	0.420	107.800	0.000	0.000
angle	3	1	16	0.420	107.800	0.000	0.000
angle	5	1	5	0.550	107.600	107.800	109.470
angle	5	1	6	0.820	110.000	108.900	108.700
angle	5	1	8	0.820	109.300	0.000	0.000
angle	5	1	9	0.760	111.000	111.000	111.000
angle	5	1	11	0.650	108.500	109.300	109.000
angle	5	1	12	0.750	105.660	106.300	107.050
angle	5	1	13	0.510	106.500	0.000	0.000
angle	5	1	14	0.620	102.800	102.800	107.800
angle	5	1	15	0.740	110.800	110.800	108.000
angle	5	1	16	0.300	108.200	0.000	0.000
angle	5	1	17	0.715	105.000	105.000	107.700
angle	5	1	18	0.690	106.000	0.000	0.000
angle	5	1	19	0.540	109.500	110.000	108.900
angle	5	1	22	0.590	109.410	109.410	109.410
angle	5	1	25	0.570	111.000	108.400	108.600
angle	5	1	26	0.498	109.938	0.000	0.000
angle	5	1	29	0.580	110.000	0.000	0.000
angle	6	1	6	0.540	103.100	101.200	107.000
angle	6	1	12	0.670	108.500	0.000	0.000
angle	6	1	22	0.830	107.500	0.000	0.000
angle	1	2	1	0.540	117.000	0.000	0.000
angle	1	2	2	0.470	122.300	0.000	0.000
angle	1	2	3	0.500	117.000	0.000	0.000
angle	1	2	4	0.470	116.600	0.000	0.000
angle	1	2	5	0.490	117.500	0.000	0.000
angle	1	2	6	0.500	120.000	0.000	0.000
angle	1	2	19	0.400	120.000	0.000	0.000

```
angle          1    3    1     1.250    116.800    116.800    116.800
angle          1    3    2     0.500    116.000      0.000      0.000
angle          1    3    3     1.000    114.600      0.000      0.000
angle          1    3    5     0.464    116.100    117.300      0.000
angle          1    3    7     0.850    123.500    123.500      0.000
angle          1    3    9     0.570    114.400      0.000      0.000
angle          1    3   11     1.950    109.000      0.000      0.000
angle          1    3   12     1.450    110.200      0.000      0.000
angle          1    3   13     1.180    109.300      0.000      0.000
angle          1    3   14     0.970    108.890      0.000      0.000
angle          2    3    2     0.850    114.700      0.000      0.000
angle          2    3    3     0.800    120.000      0.000      0.000
angle          2    3    5     0.300    111.500      0.000      0.000
angle          2    3    6     0.700    124.300      0.000      0.000
angle          2    3    7     1.300    122.000    123.500      0.000
angle          3    3    5     0.680    112.400      0.000      0.000
angle          3    3   01     0.710    121.600      0.000      0.000
angle          5    3    5     0.650    115.500      0.000      0.000
angle          5    3    6     0.550    107.000      0.000      0.000
angle          5    3    7     0.850    119.200    119.200      0.000
angle          5    3    9     0.440    109.300      0.000      0.000
angle          5    3   11     1.340    104.000      0.000      0.000
angle          5    3   12     1.220    105.150      0.000      0.000
angle          5    3   13     1.120    108.800      0.000      0.000
angle          6    3    7     1.700    121.500    122.500      0.000
angle          7    3    9     1.070    124.800      0.000      0.000
angle          7    3   22     0.460    122.500      0.000      0.000
angle          9    3    9     0.900    112.500      0.000      0.000
angle          1    6    1     0.820    107.200      0.000      0.000
angle          1    6    2     0.770    110.800      0.000      0.000
angle          1    6    3     1.250    112.800      0.000      0.000
angle          1    6    6     1.058    103.300      0.000      0.000
angle          1    6   19     0.630    117.100      0.000      0.000
angle          1    6   21     0.750    106.800      0.000      0.000
angle          1    6   25     0.770    116.000      0.000      0.000
angle          1    6   56     0.690    108.900      0.000      0.000
angle          1    6  153     1.380    119.600      0.000      0.000
angle          2    6   21     0.360    109.000      0.000      0.000
angle          2    6   25     0.800    118.000      0.000      0.000
angle          2    6   73     0.350    108.000      0.000      0.000
angle          3    6    3     0.770    106.800      0.000      0.000
angle          3    6   24     0.690    107.700      0.000      0.000
angle          3    6   56     1.250    110.800      0.000      0.000
angle          6    6   21     0.852     99.500      0.000      0.000
angle         21    6   21     0.630    105.000      0.000      0.000
angle          1   29    1     0.500    119.000      0.000      0.000
angle          1   29    5     0.420    118.000      0.000      0.000
angle          5   29    5     0.420    117.000    120.000      0.000


      ########################################
      ##                                    ##
      ##  Angle Bending Parameters (5-Ring)  ##
      ##                                    ##
      ########################################
```

```
angle5         1    1    1     0.670    109.500    109.900    111.000
angle5         1    1    2     0.540    110.200    110.200    110.600
angle5         1    1    3     0.800    111.100    111.100    111.100
angle5         1    1    6     0.770    109.300    108.400    108.400
angle5         1    1    8     0.780    109.470    108.000    109.700
angle5         1    1    9     0.750    109.480    111.900    108.500
angle5         1    1   29     0.450    110.000      0.000      0.000
angle5         2    1    2     0.540    113.200    110.000    114.500
angle5         6    1    6     0.560    106.600      0.000      0.000
angle5         1    2    1     0.540    115.200      0.000      0.000
angle5         1    2    2     0.470    122.500      0.000      0.000
angle5         1    2   37     0.550    115.100    125.000      0.000
angle5         2    2    2     0.550    121.200    121.500      0.000
angle5         2    2    6     0.600    120.000      0.000      0.000
angle5         2    2   19     0.825    120.500      0.000      0.000
angle5         1    3    1     1.250    112.700      0.000      0.000
angle5         1    3    6     1.150    111.000      0.000      0.000
angle5         1    3    9     0.620    114.400      0.000      0.000
angle5          1   29    1     0.500    119.000      0.000      0.000


      ########################################
      ##                                    ##
      ##  Angle Bending Parameters (4-Ring)  ##
      ##                                    ##
      ########################################


angle4         1    1    9     0.550    106.500      0.000      0.000
angle4         1    3    9     0.660    113.000      0.000      0.000


      ########################################
      ##                                    ##
      ##  Angle Bending Parameters (3-Ring)  ##
      ##                                    ##
      ########################################









      ##############################
      ##                          ##
      ##  Angle-Angle Parameters  ##
      ##                          ##
      ##############################


angang         1       0.240     0.300     0.000
angang         2       0.240     0.300     0.000
angang         3       0.240     0.300     0.000
angang         8       0.240     0.300     0.000
angang         9       0.240     0.300     0.000
```

```
angang        17        0.240      0.300      0.000
angang        18        0.240      0.300      0.000
angang        19        0.240      0.300      0.000
angang        22        0.240      0.300      0.000
angang        25        0.240      0.300      0.000
angang        26        0.240      0.300      0.000
angang        27        0.240      0.300      0.000
angang        29        0.240      0.300      0.000


      ################################
      ##                            ##
      ##  Stretch-Bend Parameters   ##
      ##                            ##
      ################################


   ############################################################
   ##                                                        ##
   ##          Actual MM3 Stretch-Bend Parameters            ##
   ##                                                        ##
   ##   strbnd         C        0.130      0.080      0.000   ##
   ##   strbnd         N        0.050      0.030      0.000   ##
   ##   strbnd         O        0.100      0.090      0.000   ##
   ##   strbnd         S       -0.040      0.010      0.000   ##
   ##   strbnd       P/Si       0.100      0.060      0.000   ##
   ##   strbnd         T        0.450      0.000      0.000   ##
   ##   strbnd4        C        0.050      0.080      0.000   ##
   ##   strbnd4        N        0.100      0.030      0.000   ##
   ##   strbnd4        O        0.260      0.090      0.000   ##
   ##   strbnd4        S        0.290      0.010      0.000   ##
   ##   strbnd5        C        0.130      0.080      0.000   ##
   ##   strbnd5        N        0.100      0.030      0.000   ##
   ##   strbnd5        O        0.500      0.090      0.000   ##
   ##   strbnd5        S        0.280      0.010      0.000   ##
   ##                                                        ##
   ############################################################


strbnd         1        0.130      0.080      0.000
strbnd         2        0.130      0.080      0.000
strbnd         3        0.130      0.080      0.000
strbnd         4        0.130      0.080      0.000
strbnd         6        0.100      0.090      0.000
strbnd         8        0.050      0.030      0.000
strbnd         9        0.050      0.030      0.000
strbnd        15       -0.040      0.010      0.000
strbnd        16       -0.040      0.010      0.000
strbnd        17       -0.040      0.010      0.000
strbnd        18       -0.040      0.010      0.000
strbnd        19        0.100      0.060      0.000
strbnd        22        0.130      0.080      0.000
strbnd        25        0.100      0.060      0.000
strbnd        29        0.130      0.080      0.000


      ####################################
```

```
      ##                                   ##
      ##  Out-of-Plane Bend Parameters     ##
      ##                                   ##
      #######################################


opbend        3    1          0.590
opbend        3    2          0.800
opbend        3    3          1.000
opbend        3    4          0.800
opbend        3    5          1.180
opbend        3    6          1.700
opbend        3    7          0.650
opbend        3    9          1.500
opbend        3   11          1.600
opbend        3   12          1.350
opbend        3   13          1.050
opbend        3   14          1.300
opbend        3   22          0.800
opbend        3   36          1.180
opbend        3   47          0.800
opbend        3   56          0.590
opbend        3   75          1.700
opbend        3   76          1.200
opbend        3   80          1.100
opbend        3  101          1.300
opbend        3  148          2.500
opbend        3  149          2.500


      ############################
      ##                        ##
      ##  Torsional Parameters  ##
      ##                        ##
      ############################


torsion       1   1   1   1      0.185 0.0 1     0.170 180.0 2     0.520 0.0 3
torsion       1   1   1   2      0.200 0.0 1    -0.200 180.0 2     1.300 0.0 3
torsion       1   1   1   3      0.000 0.0 1     0.400 180.0 2     0.010 0.0 3
torsion       1   1   1   4      0.200 0.0 1    -0.260 180.0 2     0.093 0.0 3
torsion       1   1   1   5      0.000 0.0 1     0.000 180.0 2     0.280 0.0 3
torsion       1   1   1   6      0.200 0.0 1     0.000 180.0 2     0.300 0.0 3
torsion       1   1   1   8     -0.302 0.0 1     0.696 180.0 2     0.499 0.0 3
torsion       1   1   1   9      0.450 0.0 1     0.000 180.0 2     0.500 0.0 3
torsion       1   1   1  11      0.780 0.0 1     0.000 180.0 2     0.300 0.0 3
torsion       1   1   1  12     -0.006 0.0 1    -0.463 180.0 2     1.145 0.0 3
torsion       1   1   1  13      0.000 0.0 1    -0.410 180.0 2     1.060 0.0 3
torsion       1   1   1  14     -1.309 0.0 1     0.440 180.0 2     0.597 0.0 3
torsion       1   1   1  15      0.000 0.0 1     0.200 180.0 2     0.400 0.0 3
torsion       1   1   1  16      0.000 0.0 1     0.000 180.0 2     0.483 0.0 3
torsion       1   1   1  17      1.500 0.0 1    -0.800 180.0 2     0.100 0.0 3
torsion       1   1   1  18     -1.500 0.0 1     0.000 180.0 2    -1.400 0.0 3
torsion       1   1   1  19      0.000 0.0 1     0.050 180.0 2     0.240 0.0 3
torsion       1   1   1  22     -0.600 0.0 1    -0.400 180.0 2     0.650 0.0 3
torsion       1   1   1  25      0.200 0.0 1     0.000 180.0 2     0.500 0.0 3
torsion       1   1   1  26     -1.238 0.0 1     0.782 180.0 2     0.201 0.0 3
torsion       1   1   1  29      0.500 0.0 1    -0.200 180.0 2     0.100 0.0 3
torsion       3   1   1   3      0.000 0.0 1     0.000 180.0 2     0.100 0.0 3
```

```
torsion      3   1   1   4      1.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      3   1   1   5      0.000 0.0 1     0.000 180.0 2     0.180 0.0 3
torsion      3   1   1   6      0.000 0.0 1     0.000 180.0 2     0.180 0.0 3
torsion      3   1   1   8      0.000 0.0 1     0.400 180.0 2     0.500 0.0 3
torsion      3   1   1   9      0.000 0.0 1     0.000 180.0 2     0.180 0.0 3
torsion      3   1   1  11     -1.000 0.0 1     0.000 180.0 2     0.200 0.0 3
torsion      3   1   1  12     -0.585 0.0 1     0.000 180.0 2     0.200 0.0 3
torsion      3   1   1  13     -0.465 0.0 1     0.000 180.0 2     0.200 0.0 3
torsion      3   1   1  15      0.000 0.0 1     0.000 180.0 2     0.483 0.0 3
torsion      3   1   1  16      0.000 0.0 1     0.000 180.0 2     0.483 0.0 3
torsion      3   1   1  25      0.000 0.0 1     0.000 180.0 2     0.400 0.0 3
torsion      3   1   1  29      0.000 0.0 1     0.000 180.0 2     0.100 0.0 3
torsion      3   1   1  36      0.000 0.0 1     0.000 180.0 2     0.180 0.0 3
torsion      3   1   1  39      0.000 0.0 1     0.400 180.0 2     0.500 0.0 3
torsion      5   1   1   5      0.000 0.0 1     0.000 180.0 2     0.238 0.0 3
torsion      5   1   1   6      0.000 0.0 1     0.000 180.0 2     0.300 0.0 3
torsion      5   1   1   8      0.000 0.0 1     0.000 180.0 2     0.374 0.0 3
torsion      5   1   1   9      0.000 0.0 1     0.000 180.0 2     0.500 0.0 3
torsion      5   1   1  11     -0.460 0.0 1     1.190 180.0 2     0.327 0.0 3
torsion      5   1   1  12      0.000 0.0 1     0.000 180.0 2     0.520 0.0 3
torsion      5   1   1  13      0.000 0.0 1     0.000 180.0 2     0.385 0.0 3
torsion      5   1   1  14      0.000 0.0 1     0.000 180.0 2     0.333 0.0 3
torsion      5   1   1  15      0.000 0.0 1     0.000 180.0 2     0.540 0.0 3
torsion      5   1   1  16      0.000 0.0 1     0.000 180.0 2     0.483 0.0 3
torsion      5   1   1  17      0.000 0.0 1     0.000 180.0 2     0.125 0.0 3
torsion      5   1   1  18      0.000 0.0 1     0.000 180.0 2     0.650 0.0 3
torsion      5   1   1  19      0.000 0.0 1     0.000 180.0 2     0.220 0.0 3
torsion      5   1   1  22      0.000 0.0 1     0.000 180.0 2     0.167 0.0 3
torsion      5   1   1  25      0.000 0.0 1     0.000 180.0 2     0.305 0.0 3
torsion      5   1   1  26      0.000 0.0 1     0.000 180.0 2     0.050 0.0 3
torsion      5   1   1  29      0.000 0.0 1     0.000 180.0 2     0.200 0.0 3
torsion     29   1   1  29      0.210 0.0 1     0.270 180.0 2     0.093 0.0 3
torsion      1   1   2   1      0.100 0.0 1     0.200 180.0 2     0.800 0.0 3
torsion      1   1   2   2     -0.700 0.0 1    -0.200 180.0 2    -0.550 0.0 3
torsion      1   1   2   3      0.000 0.0 1     0.000 180.0 2     0.457 0.0 3
torsion      1   1   2   4     -0.440 0.0 1     0.240 180.0 2     0.060 0.0 3
torsion      1   1   2   5      0.000 0.0 1     0.000 180.0 2     0.010 0.0 3
torsion      1   1   2   6      0.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      2   1   2   1     -0.900 0.0 1     0.000 180.0 2    -0.300 0.0 3
torsion      2   1   2   2      0.250 0.0 1    -0.650 180.0 2     0.600 0.0 3
torsion      2   1   2   5      0.000 0.0 1     0.000 180.0 2     0.800 0.0 3
torsion      2   1   2   6      0.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      3   1   2   1      0.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      3   1   2   2      0.000 0.0 1     0.000 180.0 2     0.100 0.0 3
torsion      3   1   2   5      0.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      5   1   2   1      0.000 0.0 1     0.000 180.0 2     0.540 0.0 3
torsion      5   1   2   2      0.000 0.0 1     0.000 180.0 2    -0.090 0.0 3
torsion      5   1   2   3      0.000 0.0 1     0.000 180.0 2     0.274 0.0 3
torsion      5   1   2   4      0.000 0.0 1     0.000 180.0 2    -0.240 0.0 3
torsion      5   1   2   5      0.000 0.0 1     0.000 180.0 2     0.580 0.0 3
torsion      5   1   2   6      0.000 0.0 1     0.000 180.0 2     0.540 0.0 3
torsion      1   1  29   1      0.400 0.0 1     0.150 180.0 2     0.500 0.0 3
torsion      1   1  29   5      0.000 0.0 1     0.200 180.0 2     0.300 0.0 3
torsion      5   1  29   1      0.000 0.0 1     0.000 180.0 2     0.280 0.0 3
torsion      5   1  29   5      0.000 0.0 1     0.000 180.0 2     0.300 0.0 3
torsion      6   1   2   1      0.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      6   1   2   2     -0.500 0.0 1     1.000 180.0 2    -0.985 0.0 3
torsion      6   1   2   5      0.000 0.0 1     0.000 180.0 2     0.000 0.0 3
torsion      1   1   3   1      0.406 0.0 1     0.292 180.0 2     0.014 0.0 3
torsion      1   1   3   2      0.000 0.0 1     0.000 180.0 2    -0.110 0.0 3
torsion      1   1   3   5      0.655 0.0 1     0.266 180.0 2     0.474 0.0 3
torsion      1   1   3   6      0.550 0.0 1     1.550 180.0 2     0.100 0.0 3
torsion      1   1   3   7     -0.457 0.0 1     1.106 180.0 2    -0.160 0.0 3
```

torsion	2	1	3	1	0.000	0.0	1	0.000	180.0	2	0.000	0.0 3
torsion	2	1	3	2	2.100	0.0	1	1.200	180.0	2	-0.900	0.0 3
torsion	2	1	3	5	0.000	0.0	1	0.000	180.0	2	0.000	0.0 3
torsion	2	1	3	6	0.000	0.0	1	0.000	180.0	2	-0.417	0.0 3
torsion	2	1	3	7	0.000	0.0	1	0.000	180.0	2	-0.350	0.0 3
torsion	2	1	3	9	3.410	0.0	1	0.663	180.0	2	-0.150	0.0 3
torsion	3	1	3	1	0.000	0.0	1	0.000	180.0	2	0.000	0.0 3
torsion	3	1	3	5	0.000	0.0	1	0.000	180.0	2	0.000	0.0 3
torsion	3	1	3	7	0.000	0.0	1	0.000	180.0	2	-0.350	0.0 3
torsion	3	1	3	9	3.299	0.0	1	-1.450	180.0	2	-2.300	0.0 3
torsion	5	1	3	1	0.000	0.0	1	0.000	180.0	2	0.150	0.0 3
torsion	5	1	3	2	0.000	0.0	1	0.000	180.0	2	-0.140	0.0 3
torsion	5	1	3	3	0.000	0.0	1	0.000	180.0	2	0.500	0.0 3
torsion	5	1	3	5	0.115	0.0	1	0.027	180.0	2	0.285	0.0 3
torsion	5	1	3	6	0.250	0.0	1	0.850	180.0	2	0.000	0.0 3
torsion	5	1	3	7	-0.154	0.0	1	0.044	180.0	2	-0.086	0.0 3
torsion	5	1	3	9	0.000	0.0	1	0.000	180.0	2	0.230	0.0 3
torsion	5	1	3	11	0.000	0.0	1	0.000	180.0	2	0.192	0.0 3
torsion	5	1	3	12	0.000	0.0	1	0.000	180.0	2	0.219	0.0 3
torsion	5	1	3	13	0.000	0.0	1	0.000	180.0	2	0.195	0.0 3
torsion	5	1	3	14	0.000	0.0	1	0.000	180.0	2	0.160	0.0 3
torsion	1	2	2	1	-0.300	0.0	1	9.500	180.0	2	0.000	0.0 3
torsion	1	2	2	2	-0.610	0.0	1	7.000	180.0	2	0.000	0.0 3
torsion	1	2	2	3	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	1	2	2	5	0.000	0.0	1	10.000	180.0	2	0.000	0.0 3
torsion	2	2	2	2	-0.670	0.0	1	10.000	180.0	2	0.000	0.0 3
torsion	2	2	2	3	0.000	0.0	1	10.000	180.0	2	0.000	0.0 3
torsion	2	2	2	4	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	2	2	2	5	0.250	0.0	1	9.000	180.0	2	-0.550	0.0 3
torsion	2	2	2	6	0.000	0.0	1	16.250	180.0	2	0.000	0.0 3
torsion	3	2	2	3	0.000	0.0	1	8.700	180.0	2	0.000	0.0 3
torsion	3	2	2	5	0.000	0.0	1	10.400	180.0	2	0.000	0.0 3
torsion	3	2	2	8	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	5	0.000	0.0	1	11.500	180.0	2	0.000	0.0 3
torsion	5	2	2	6	0.000	0.0	1	16.250	180.0	2	0.000	0.0 3
torsion	5	2	2	8	0.000	0.0	1	9.000	180.0	2	0.000	0.0 3
torsion	5	2	2	9	0.000	0.0	1	12.000	180.0	2	0.000	0.0 3
torsion	5	2	2	11	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	12	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	13	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	14	-1.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	18	0.000	0.0	1	8.380	180.0	2	0.300	0.0 3
torsion	5	2	2	19	0.000	0.0	1	6.450	180.0	2	0.000	0.0 3
torsion	5	2	2	22	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	25	0.000	0.0	1	16.250	180.0	2	0.000	0.0 3
torsion	5	2	2	26	0.000	0.0	1	11.600	180.0	2	0.000	0.0 3
torsion	5	2	2	37	0.755	0.0	1	10.000	180.0	2	0.000	0.0 3
torsion	5	2	2	39	0.000	0.0	1	15.000	180.0	2	0.000	0.0 3
torsion	5	2	2	40	-3.150	0.0	1	3.000	180.0	2	0.000	0.0 3
torsion	5	2	2	41	-0.250	0.0	1	10.000	180.0	2	0.000	0.0 3
torsion	5	2	2	42	-4.242	0.0	1	7.400	180.0	2	0.000	0.0 3
torsion	5	2	2	43	0.000	0.0	1	14.000	180.0	2	-1.060	0.0 3
torsion	5	2	2	46	0.000	0.0	1	8.500	180.0	2	0.000	0.0 3
torsion	5	2	2	57	0.250	0.0	1	9.000	180.0	2	-0.550	0.0 3
torsion	5	2	2	111	0.000	0.0	1	12.620	180.0	2	-1.100	0.0 3
torsion	5	2	2	143	0.000	0.0	1	12.800	180.0	2	-1.060	0.0 3
torsion	5	2	2	144	0.000	0.0	1	14.000	180.0	2	0.000	0.0 3
torsion	1	2	3	1	0.980	0.0	1	10.379	180.0	2	0.000	0.0 3
torsion	1	2	3	2	0.000	0.0	1	9.820	180.0	2	0.000	0.0 3
torsion	1	2	3	5	3.250	0.0	1	12.000	180.0	2	0.000	0.0 3
torsion	1	2	3	7	2.020	0.0	1	12.000	180.0	2	0.000	0.0 3
torsion	1	2	3	151	3.804	0.0	1	9.139	180.0	2	-1.199	0.0 3
torsion	5	2	3	1	0.000	0.0	1	8.000	180.0	2	0.000	0.0 3

```
torsion        5   2   3   2       0.400 0.0 1      9.820 180.0 2      0.000 0.0 3
torsion        5   2   3   3       0.000 0.0 1      9.800 180.0 2      0.000 0.0 3
torsion        5   2   3   5       2.750 0.0 1     10.000 180.0 2      0.000 0.0 3
torsion        5   2   3   7       2.100 0.0 1     10.000 180.0 2      0.000 0.0 3
torsion        1   3   3   1       1.000 0.0 1      6.500 180.0 2      0.000 0.0 3
torsion        1   3   3   5       0.000 0.0 1      5.200 180.0 2      0.000 0.0 3
torsion        1   3   3  76      -1.000 0.0 1      6.500 180.0 2      0.000 0.0 3
torsion        2   3   3   2       0.900 0.0 1      8.000 180.0 2      0.000 0.0 3
torsion        2   3   3   5       0.000 0.0 1      5.000 180.0 2      0.000 0.0 3
torsion        2   3   3  76      -1.500 0.0 1      3.000 180.0 2      0.000 0.0 3
torsion        5   3   3   5      -0.700 0.0 1      9.800 180.0 2      0.000 0.0 3


      ######################################
      ##                                  ##
      ##  Torsional Parameters (5-Ring)   ##
      ##                                  ##
      ######################################


torsion5       1   1   1   1       0.185 0.0 1      0.170 180.0 2      1.160 0.0 3
torsion5       1   1   1   1       0.185 0.0 1      0.170 180.0 2      1.160 0.0 3
torsion5       1   1   1   2       0.225 0.0 1      0.410 180.0 2      1.150 0.0 3
torsion5       1   1   1   3       0.000 0.0 1      0.400 180.0 2      1.620 0.0 3
torsion5       1   1   1   6       0.300 0.0 1      0.000 180.0 2      1.800 0.0 3
torsion5       1   1   1   8      -0.302 0.0 1      0.696 180.0 2      1.360 0.0 3
torsion5       1   1   1   9       0.450 0.0 1      0.000 180.0 2      0.500 0.0 3
torsion5       1   1   1  15       0.000 0.0 1      0.200 180.0 2      2.150 0.0 3
torsion5       1   1   1  18      -1.500 0.0 1      0.320 180.0 2      0.100 0.0 3
torsion5       1   1   1  19       0.000 0.0 1      0.000 180.0 2      0.850 0.0 3
torsion5       1   1   1  22       0.450 0.0 1     -0.750 180.0 2      0.350 0.0 3
torsion5       1   1   1  29       0.400 0.0 1      1.200 180.0 2      0.500 0.0 3
torsion5       1   1   1  37       0.200 0.0 1      0.600 180.0 2      0.100 0.0 3
torsion5       1   1   1  56       0.185 0.0 1      0.170 180.0 2      1.160 0.0 3
torsion5       1   1   1  57       0.185 0.0 1      0.170 180.0 2      1.160 0.0 3
torsion5       2   1   1   2       0.000 0.0 1      0.000 180.0 2      0.000 0.0 3
torsion5       2   1   1  19       0.000 0.0 1      0.000 180.0 2      0.167 0.0 3
torsion5       3   1   1   3       0.000 0.0 1      0.000 180.0 2      0.180 0.0 3
torsion5       3   1   1   6       0.000 0.0 1      0.000 180.0 2      0.000 0.0 3
torsion5       1   1   2   1      -0.100 0.0 1      0.030 180.0 2      1.350 0.0 3
torsion5       1   1   2   2      -0.900 0.0 1     -0.900 180.0 2      0.300 0.0 3
torsion5       1   1   2  37       0.000 0.0 1      0.000 180.0 2     -0.250 0.0 3
torsion5       2   1   2   1       0.000 0.0 1      0.000 180.0 2      0.000 0.0 3
torsion5       2   1   2   2       0.250 0.0 1     -0.400 180.0 2     -0.500 0.0 3
torsion5       2   1   2  37       0.000 0.0 1      0.000 180.0 2      0.000 0.0 3
torsion5       9   1   2   6      -0.100 0.0 1      0.990 180.0 2     -0.800 0.0 3
torsion5       1   1   3   1       0.606 0.0 1      0.292 180.0 2      1.220 0.0 3
torsion5       1   1   3   6       1.050 0.0 1      1.106 180.0 2      0.000 0.0 3
torsion5       1   1  29   1       0.600 0.0 1      3.500 180.0 2      1.200 0.0 3


      ######################################
      ##                                  ##
      ##  Torsional Parameters (4-Ring)   ##
      ##                                  ##
      ######################################


torsion4       3   1   1   9       0.000 0.0 1      0.000 180.0 2      0.250 0.0 3
torsion4       1   1   3   9       0.000 0.0 1      0.000 180.0 2      0.250 0.0 3
torsion4       1   1   9   3       0.000 0.0 1      0.000 180.0 2      0.250 0.0 3
torsion4       1   3   9   1       0.000 0.0 1      0.000 180.0 2      0.250 0.0 3
```

```
      ###################################
      ##                                 ##
      ##  Stretch Torsion Parameters     ##
      ##                                 ##
      ###################################


strtors       1    1          0.000      0.000      0.059
strtors       1    2          0.000      0.000      0.270
strtors       1    3          0.000      0.000      0.100
strtors       1    6          0.000      0.000      0.100
strtors       6    6          0.000      0.000      0.220

      ######################################
      ##                                  ##
      ##  Bond Dipole Moment Parameters   ##
      ##                                  ##
      ######################################


dipole        1    2         0.9000      0.500
dipole        1    3         1.0100      0.500
dipole        1    4         1.6400      0.500
dipole        1    5         0.0000      0.500
dipole        1    6         1.1700      0.500
dipole        1    8         0.6800      0.500
dipole        3    5        -0.6000      0.500
dipole        3    6         0.1200      0.500
dipole        3    7         1.8600      0.500



      ############################################
      ##                                        ##
      ##  Conjugated Pisystem Atom Parameters   ##
      ##                                        ##
      ############################################


piatom        2         1.0      -11.160     11.134
piatom        3         1.0      -11.160     11.134
piatom        4         1.0      -11.160     11.134
piatom        6         2.0      -14.533     19.342
piatom        7         1.0      -16.646     14.520


      ############################################
      ##                                        ##
      ##  Conjugated Pisystem Bond Parameters   ##
      ##                                        ##
      ############################################
```

```
pibond        2    2          2.820      0.1700
pibond        2    3          4.600      0.1660
pibond        2    4          7.790      0.1560
pibond        3    3          8.000      0.3500
pibond        3    4          4.600      0.1660
pibond        3    7          6.350      0.3000


      ##################################################
      ##                                              ##
      ##  Conjugated Pisystem Bond Parameters (5-Ring)  ##
      ##                                              ##
      ##################################################


pibond5       2    2          4.020      0.1690
pibond5       2    3          4.600      0.1660
pibond5       2   37          8.250      0.2380
pibond5       2   40          6.300      0.1960
pibond5       2   41          8.200      0.1620
pibond5       2   42          4.861      0.2000
pibond5       3    3          4.600      0.1660
pibond5       3   57          4.600      0.1660
pibond5      37   37          9.100      0.2800
pibond5      37   40          8.000      0.1960
pibond5      37   41          5.120      0.1700
pibond5      37   42          4.861      0.3970
pibond5      57   57          2.820      0.1700


      ##################################################
      ##                                              ##
      ##  Conjugated Pisystem Bond Parameters (4-Ring)  ##
      ##                                              ##
      ##################################################


pibond4      57   57          2.840      0.3900
pibond4      57   58          4.600      0.1660
pibond4      58   58          4.600      0.1660

#new parameters
atom   20     O     "O in OH radical"   8  15.995  1
dipole        20   21        -1.6700      0.500
vdw           20              1.820       0.059
bond          20   21         4.71        0.9707
bond          1    5         4.7400      1.1120
bond          6   21         7.6300     0.9470

#new parameters
atom   122   O   "Atomic Oxygen"   8   15.995   0
vdw           122              1.820       0.059
```