Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Conformational changes in hydroxyl functional group upon hydration: the case study of Endo Fenchol

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EF-OH:H_2O

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-------------------------------------------------------------------------------
=========
                                                obs         o-c     error     blends
Notes
                                                                              o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------
=========
   1:  7  0  7    6  0  6                      9000.9709  -0.0009  0.002
   2:  7  1  7    6  1  6                      8982.5334  -0.0005  0.002
   3:  6  0  6    5  0  5                      7765.7572  -0.0011  0.002
   4:  6  1  6    5  1  5                      7729.3502  -0.0008  0.002
   5:  5  0  5    4  0  4                      6533.9642  -0.0012  0.002
   6:  5  1  5    4  1  4                      6469.1748   0.0002  0.002
   7:  8  1  8    7  1  7                     10231.4772  -0.0004  0.002
   8:  8  0  8    7  0  7                     10240.2154  -0.0004  0.002
   9:  9  0  9    8  0  8                     11482.0684  -0.0004  0.002
  10:  9  1  9    8  1  8                     11478.1076  -0.0004  0.002
  11: 10  1 10    9  1  9                     12723.5766   0.0000  0.002
  12: 10  0 10    9  0  9                     12725.3153  -0.0002  0.002
  13: 11  0 11   10  0 10                     13969.2430   0.0000  0.002
  14:  8  2  7    7  2  6                     10734.7568  -0.0004  0.002
  15: 11  1 11   10  1 10                     13968.4972  -0.0002  0.002
  16:  4  0  4    3  0  3                      5296.9459  -0.0012  0.002
  17:  4  1  4    3  1  3                      5198.8579  -0.0005  0.002
  18:  3  0  3    2  0  2                      4034.0966   0.0011  0.002
  19:  5  1  4    4  1  3                      7066.4668   0.0000  0.002
  20:  4  1  3    3  1  2                      5704.4056   0.0000  0.002
  21:  6  1  5    5  1  4                      8378.5576   0.0017  0.002
  22:  6  2  5    5  2  4                      8145.1689   0.0001  0.002
  23:  7  0  7    6  1  6                      8966.8170  -0.0006  0.002
  24:  7  1  7    6  0  6                      9016.6870  -0.0011  0.002
  25:  6  3  4    5  3  3                      8320.3853   0.0014  0.002
  26:  5  2  3    4  2  2                      7162.6016  -0.0001  0.002
  27:  5  3  2    4  3  1                      6989.1854   0.0002  0.002
  28:  5  3  3    4  3  2                      6933.6921  -0.0003  0.002
  29:  5  2  4    4  2  3                      6822.6193   0.0005  0.002
  30:  4  2  2    3  2  1                      5685.6717   0.0007  0.002
  31:  4  2  3    3  2  2                      5481.9714  -0.0004  0.002
  32:  3  1  2    2  1  1                      4304.7731   0.0007  0.002
  33:  7  2  6    6  2  5                      9448.8147  -0.0004  0.002
  34:  7  3  5    6  3  4                      9695.8995   0.0003  0.002
  35:  7  4  4    6  4  3                      9735.5071  -0.0003  0.002
  36:  7  5  3    6  5  2                      9713.1161  -0.0001  0.002
  37:  7  5  2    6  5  1                      9714.4250   0.0011  0.002
  38:  7  3  4    6  3  3                      9951.0608   0.0011  0.002
  39:  7  2  5    6  2  4                     10043.8701   0.0003  0.002
  40:  8  1  7    7  1  6                     10868.3205  -0.0005  0.002
  41:  5  2  3    4  1  3                      8454.5954   0.0016  0.002
  42:  6  3  3    5  3  2                      8454.3044   0.0032  0.002
  43:  8  3  6    7  3  5                     11055.0265   0.0002  0.002
  44:  8  3  5    7  3  4                     11457.5664   0.0010  0.002
  45:  8  2  6    7  2  5                     11418.6209   0.0003  0.002
  46:  8  4  4    7  4  3                     11218.4793   0.0011  0.002
  47:  8  4  5    7  4  4                     11140.9908   0.0003  0.002
  48:  8  5  3    7  5  2                     11125.0532   0.0010  0.002
  49:  9  1  8    8  1  7                     12087.3934  -0.0007  0.002
  50:  9  2  8    8  2  7                     12005.9325   0.0037  0.002
  51:  9  3  7    8  3  6                     12394.2326  -0.0001  0.002
  52:  6  2  4    5  2  3                      8621.1611   0.0005  0.002
  53:  9  5  5    8  5  4                     12532.6141   0.0006  0.002
  54:  9  1  9    8  0  8                     11485.0855  -0.0006  0.002
  55/  7  2  5    6  1  5                     11674.5913  -0.0102  0.002
  56:  7  3  4    6  2  4                     12001.1627   0.0004  0.002
  57:  9  6  4    8  6  3                     12498.8479   0.0018  0.002
  58:  9  4  6    8  4  5                     12541.5453   0.0008  0.002
  59:  9  5  4    8  5  3                     12548.3935   0.0000  0.002
  60:  7  3  5    6  2  5                     12672.4705   0.0015  0.002
  61:  9  4  5    8  4  4                     12705.5284   0.0010  0.002
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  62:  9  2  7    8  2  6                  12736.0579   0.0000  0.002
  63:  9  3  6    8  3  5                  12944.1545   0.0007  0.002
  64: 10  2  9    9  2  8                  13266.1400  -0.0002  0.002
  65: 10  1  9    9  1  8                  13311.0790  -0.0004  0.002
  66:  8  3  5    7  2  5                  13414.8585   0.0006  0.002
  67: 10  3  8    9  3  7                  13712.1219   0.0000  0.002
  68: 10  6  5    9  6  4                  13909.6784   0.0002  0.002
  69: 10  6  4    9  6  3                  13912.2394  -0.0004  0.002
  70: 10  4  7    9  4  6                  13931.0427   0.0004  0.002
  71: 10  5  5    9  5  4                  13990.5196   0.0006  0.002
  72: 10  4  6    9  4  5                  14224.9612   0.0009  0.002
  73/ 10  5  6    9  5  5                  13949.1468  -0.0098  0.002
  74: 10  3  7    9  3  6                  14388.7102   0.0003  0.002
  75:  7  5  3    6  4  3                  14355.3523   0.0002  0.002
  76:  7  5  2    6  4  2                  14344.8621   0.0003  0.002
  77: 11  2 10   10  2  9                  14519.0851   0.0000  0.002
  78: 11  1 10   10  1  9                  14542.1985  -0.0003  0.002
  79: 11  3  9   10  3  8                  15009.5409  -0.0004  0.002
  80: 12  1 12   11  1 11                  15213.1723   0.0005  0.002
  81: 12  0 12   11  0 11                  15213.4859   0.0005  0.002
  82: 11  2  9   10  2  8                  15216.5568  -0.0005  0.002
  83: 11  4  7   10  4  6                  15756.4319   0.0011  0.002
  84: 11  3  8   10  3  7                  15777.6902   0.0000  0.002
  85:  7  4  4    6  3  4                  13368.6980   0.0003  0.002
  86:  7  4  3    6  3  3                  13202.2872  -0.0006  0.002
  87:  6  4  3    5  3  3                  11953.5747   0.0006  0.002
  88:  6  4  2    5  3  2                  11890.5913   0.0001  0.002
  89:  7  6  1    6  5  1                  15393.8842   0.0000  0.002
  90: 11  4  8   10  4  7                  15303.8528   0.0005  0.002
  91: 12  1 11   11  1 10                  15779.0001   0.0010  0.002
  92:  7  7  1    6  6  0                  16433.2982   0.0006  0.002  -0.0004 0.50
  93:  7  7  0    6  6  1                  16433.2982  -0.0014  0.002  -0.0004 0.50
  94:  5  5  1    4  4  1                  11589.8147  -0.0007  0.002
  95:  5  5  0    4  4  0                  11589.5630   0.0011  0.002
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PARAMETERS IN FIT (values truncated):

       10000            A  /MHz         1210.91653(16)                        1
       20000            B  /MHz          752.900591(88)                       2
       30000            C  /MHz          622.335817(68)                       3
         200      DELTA J  /kHz            0.08308(35)                        4
        2000      DELTA K  /kHz           -0.1445(33)                         5
        1100     DELTA JK  /kHz            0.2412(20)                        6
       40100      delta J  /kHz            0.01321(19)                        7
       41000      delta K  /kHz            0.0619(37)                         8

 MICROWAVE AVG =        0.000013 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001709 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.85455         0.85455

  distinct frequency lines in fit:    94
       distinct parameters of fit:     8

                                  upper state  lower state         overall
      limits of quantum number  1:      3   12       2   11           2   12
      limits of quantum number  2:      0    7       0    6           0    7
      limits of quantum number  3:      0   12       0   11           0   12

                  frequency range:        4034        16433

 Standard errors are obtained by muliplying the previous errors by:   0.893413

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000            A  /MHz         1210.91654(14)                        1
       20000            B  /MHz          752.900591(78)                       2
       30000            C  /MHz          622.335817(60)                       3
         200      DELTA J  /kHz            0.08308(31)                        4
        2000      DELTA K  /kHz           -0.1445(29)                         5
        1100     DELTA JK  /kHz            0.2413(18)                        6
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        40100      delta J  /kHz            0.01322(17)                          7
        41000      delta K  /kHz            0.0619(33)                           8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DELTA J -DELTA K -DELTA J -delta J -delta K

A           1.0000
B           0.0170   1.0000
C          -0.0415  -0.4358   1.0000
-DELTA J    0.1069  -0.7207   0.0549   1.0000
-DELTA K   -0.6181   0.0382   0.1629   0.1306   1.0000
-DELTA JK  -0.3040   0.1087  -0.2289  -0.5208  -0.4374   1.0000
-delta J    0.0746  -0.8311   0.6782   0.5981   0.0904  -0.3538   1.0000
-delta K   -0.0053  -0.5390   0.4279   0.7192   0.1849  -0.4548   0.4982   1.0000

 Mean value of |C.ij|, i.ne.j =   0.3351
 Mean value of  C.ij,  i.ne.j =  -0.0572


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    55:   -5.1         73:   -4.9         50:    1.9         42:    1.6
    57:    0.9         21:    0.8         41:    0.8         60:    0.8
    25:    0.7         16:   -0.6          5:   -0.6         95:    0.6
    38:    0.6         37:    0.6         18:    0.6          3:   -0.6
    83:    0.6         24:   -0.6         46:    0.6         61:    0.5
    48:    0.5         44:    0.5         91:    0.5          1:   -0.4
    72:    0.4         58:    0.4          4:   -0.4         94:   -0.3
    49:   -0.3         30:    0.3         63:    0.3         32:    0.3
    54:   -0.3         71:    0.3         66:    0.3         53:    0.3
    23:   -0.3         87:    0.3         86:   -0.3         80:    0.2
    52:    0.2         90:    0.2         40:   -0.2         29:    0.2
    17:   -0.2          2:   -0.2         82:   -0.2         81:    0.2
    69:   -0.2         92:   -0.2

    55/  7  2  5    6  1  5                    11674.5913  -0.0102  0.002
    73/ 10  5  6    9  5  5                    13949.1468  -0.0098  0.002
    50:  9  2  8    8  2  7                    12005.9325   0.0037  0.002
    42:  6  3  3    5  3  2                     8454.3044   0.0032  0.002
    57:  9  6  4    8  6  3                    12498.8479   0.0018  0.002
    21:  6  1  5    5  1  4                     8378.5576   0.0017  0.002
    41:  5  2  3    4  1  3                     8454.5954   0.0016  0.002
    60:  7  3  5    6  2  5                    12672.4705   0.0015  0.002
    25:  6  3  4    5  3  3                     8320.3853   0.0014  0.002
    16:  4  0  4    3  0  3                     5296.9459  -0.0012  0.002

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_____________________________________________/ SPFIT output reformatted with PIFORM
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EF-OD:D_2O

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------------------------------------------------------------------------------
=========
                                                obs         o-c     error     blends
Notes
                                                                          o-c      wt
    / instead of : below denotes (o-c)>3*err
------------------------------------------------------------------------------
=========
   1:  4  0  4     3  0  3                      5105.7394  -0.0017  0.002
   2:  4  1  4     3  1  3                      5005.3666  -0.0028  0.002
   3:  5  0  5     4  0  4                      6300.9955   0.0029  0.002
   4:  5  1  5     4  1  4                      6230.7973  -0.0013  0.002
   5:  6  1  6     5  1  5                      7446.6931  -0.0014  0.002
   6:  6  0  6     5  0  5                      7488.4973  -0.0017  0.002
   7:  7  1  7     6  1  6                      8655.6773  -0.0002  0.002
   8:  7  0  7     6  0  6                      8678.0583   0.0020  0.002
   9:  8  1  8     7  1  7                      9860.2325   0.0018  0.002
  10:  8  0  8     7  0  7                      9871.4150   0.0025  0.002
  11:  9  0  9     8  0  8                     11067.5545  -0.0012  0.002
  12:  9  1  9     8  1  8                     11062.2211   0.0000  0.002
  13: 10  1 10     9  1  9                     12262.8437  -0.0021  0.002
  14: 10  0 10     9  0  9                     12265.3077  -0.0009  0.002
  15: 11  1 11    10  1 10                     13462.7895   0.0017  0.002
  16: 11  0 11    10  0 10                     13463.8995   0.0023  0.002
  17: 12  1 12    11  1 11                     14662.3995  -0.0046  0.002
  18: 12  0 12    11  0 11                     14662.8977   0.0032  0.002
  19:  6  1  5     5  1  4                      8067.1104   0.0001  0.002
  20:  6  3  4     5  3  3                      7986.8900   0.0009  0.002
  21:  6  2  4     5  2  3                      8263.4176   0.0028  0.002
  22:  7  2  5     6  2  4                      9638.5526  -0.0029  0.002
  23:  8  2  7     7  2  6                     10335.9773  -0.0012  0.002
  24:  8  1  7     7  1  6                     10485.8781   0.0032  0.002
  25:  8  3  6     7  3  5                     10621.6917   0.0004  0.002
  26:  9  1  8     8  1  7                     11662.4694  -0.0028  0.002
------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000            A  /MHz         1192.7851(22)                         1
        20000            B  /MHz          721.01710(17)                        2
        30000            C  /MHz          599.76547(10)                        3
          200         DelJ  /kHz            0.08088(48)                        4
         1100        DelJK  /kHz            0.198(17)                          5
         2000      DELTA K  /kHz          [-0.144453483]                       6
        40100      delta J  /kHz          [ 0.013217235]                       7
        41000      delta K  /kHz          [ 0.061912479]                       8

 MICROWAVE AVG =       -0.000046 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002199 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        1.09951         1.09951

  distinct frequency lines in fit:    26
       distinct parameters of fit:     5

                                  upper state  lower state         overall
      limits of quantum number  1:      4   12       3   11           3   12
      limits of quantum number  2:      0    3       0    3           0    3
      limits of quantum number  3:      4   12       3   11           3   12

                 frequency range:        5005        14662

 Standard errors are obtained by muliplying the previous errors by:   1.223422

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

        10000            A  /MHz         1192.7852(28)                         1
        20000            B  /MHz          721.01711(21)                        2
        30000            C  /MHz          599.76547(12)                        3
```

```
          200         DelJ  /kHz            0.08088(58)                        4
         1100        DelJK  /kHz            0.198(21)                          5
         2000      DELTA K  /kHz          [-0.144453483]                       6
        40100      delta J  /kHz          [ 0.013217235]                       7
        41000      delta K  /kHz          [ 0.061912479]                       8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DelJ    -DelJK

A           1.0000
B           0.3882   1.0000
C          -0.5694  -0.2269   1.0000
-DelJ       0.5417   0.4004  -0.8570   1.0000
-DelJK     -0.6067  -0.7339   0.2154  -0.5468   1.0000

 Mean value of |C.ij|, i.ne.j =   0.5086
 Mean value of  C.ij,  i.ne.j =  -0.1995


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    17:   -2.3         24:    1.6         18:    1.6          3:    1.4
    22:   -1.4         26:   -1.4         21:    1.4          2:   -1.4
    10:    1.2         16:    1.1         13:   -1.0          8:    1.0
     9:    0.9          1:   -0.8         15:    0.8          6:   -0.8
     5:   -0.7          4:   -0.6         11:   -0.6         23:   -0.6
    14:   -0.4         20:    0.4         25:    0.2          7:   -0.1
    19:    0.1         12:    0.0

    17: 12  1 12   11  1 11                    14662.3995  -0.0046  0.002
    24:  8  1  7    7  1  6                    10485.8781   0.0032  0.002
    18: 12  0 12   11  0 11                    14662.8977   0.0032  0.002
     3:  5  0  5    4  0  4                     6300.9955   0.0029  0.002
    22:  7  2  5    6  2  4                     9638.5526  -0.0029  0.002
    26:  9  1  8    8  1  7                    11662.4694  -0.0028  0.002
    21:  6  2  4    5  2  3                     8263.4176   0.0028  0.002
     2:  4  1  4    3  1  3                     5005.3666  -0.0028  0.002
    10:  8  0  8    7  0  7                     9871.4150   0.0025  0.002
    16: 11  0 11   10  0 10                    13463.8995   0.0023  0.002

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EF-OD:HOD

```
-------------------------------------------------------------------------------
=========
                                                obs         o-c     error     blends
Notes
                                                                          o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------
=========
   1:  5  1  5    4  1  4                      6297.2644   0.0005  0.002
   2:  6  1  6    5  1  5                      7525.7130  -0.0008  0.002
   3:  7  1  7    6  1  6                      8747.2459   0.0000  0.002
   4:  8  1  8    7  1  7                      9964.4077   0.0007  0.002
   5:  8  0  8    7  0  7                      9974.8874  -0.0001  0.002
   6:  9  1  9    8  1  8                     11179.0767  -0.0005  0.002
   7:  9  0  9    8  0  8                     11184.0130   0.0002  0.002
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

       10000            A  /MHz         1195.996(71)                          1
       20000            B  /MHz          729.320(11)                          2
       30000            C  /MHz          606.1714(30)                         3
         200      DELTA J  /kHz            0.0524(81)                         4
        1100        DelJK  /kHz          [ 0.858790325]                       5
        2000         DelK  /kHz          [ 0.056690297]                       6
       40100         delJ  /kHz          [ 0.00625862104]                     7
       41000         delK  /kHz          [ 0.136393167]                       8

 MICROWAVE AVG =        0.000002 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000522 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.26113         0.26113

  distinct frequency lines in fit:     7
       distinct parameters of fit:     4

                                    upper state  lower state         overall
      limits of quantum number  1:      5    9       4    8           4    9
      limits of quantum number  2:      0    1       0    1           0    1
      limits of quantum number  3:      5    9       4    8           4    9

                  frequency range:        6297        11184

 Standard errors are obtained by muliplying the previous errors by:   0.398883

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000            A  /MHz         1195.996(28)                          1
       20000            B  /MHz          729.3201(45)                         2
       30000            C  /MHz          606.1714(12)                         3
         200      DELTA J  /kHz            0.0524(32)                         4
        1100        DelJK  /kHz          [ 0.858790325]                       5
        2000         DelK  /kHz          [ 0.056690297]                       6
       40100         delJ  /kHz          [ 0.00625862104]                     7
       41000         delK  /kHz          [ 0.136393167]                       8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DELTA J

A           1.0000
B           0.9062   1.0000
C          -0.9525  -0.9880   1.0000
-DELTA J    0.8797   0.9813  -0.9803   1.0000

 Mean value of |C.ij|, i.ne.j =   0.9480
 Mean value of  C.ij,  i.ne.j =  -0.0256
 No correlations with absolute value greater than 0.9950
```

Worst fitted lines (obs-calc/error):

2: -0.4	4: 0.3	1: 0.2	6: -0.2
7: 0.1	5: -0.1	3: 0.0	

2:	6	1	6	5	1	5	7525.7130	-0.0008	0.002
4:	8	1	8	7	1	7	9964.4077	0.0007	0.002
1:	5	1	5	4	1	4	6297.2644	0.0005	0.002
6:	9	1	9	8	1	8	11179.0767	-0.0005	0.002
7:	9	0	9	8	0	8	11184.0130	0.0002	0.002
5:	8	0	8	7	0	7	9974.8874	-0.0001	0.002
3:	7	1	7	6	1	6	8747.2459	0.0000	0.002

/ SPFIT output reformatted with PIFORM

EF-OH:D_2O

```
--------------------------------------------------------------------------------
=========
                                                obs         o-c     error     blends
Notes
                                                                              o-c      wt
    / instead of : below denotes (o-c)>3*err
--------------------------------------------------------------------------------
=========
   1:  8  1  8     7  1  7                      9881.4978   0.0019  0.002
   2:  8  0  8     7  0  7                      9892.6754   0.0017  0.002
   3:  9  1  9     8  1  8                     11085.5815   0.0017  0.002
   4:  9  0  9     8  0  8                     11090.8943  -0.0011  0.002
   5: 10  1 10     9  1  9                     12288.2916   0.0003  0.002
   6: 10  0 10     9  0  9                     12290.7375  -0.0002  0.002
   7:  6  1  6     5  1  5                      7463.6738   0.0002  0.002
   8:  6  0  6     5  0  5                      7505.7448  -0.0016  0.002
   9:  5  0  5     4  0  4                      6316.3959  -0.0014  0.002
  10:  5  1  5     4  1  4                      6245.4937  -0.0032  0.002
  11:  7  1  7     6  1  6                      8674.8274   0.0003  0.002
  12:  6  1  5     5  1  4                      8095.1577  -0.0002  0.002
  13:  6  2  4     5  2  3                      8297.1771  -0.0008  0.002
  14:  8  3  5     7  3  4                     11007.9533  -0.0026  0.002
  15:  8  2  6     7  2  5                     11016.6365   0.0031  0.002
  16:  9  1  8     8  1  7                     11695.2741  -0.0012  0.002
  17: 10  1  9     9  1  8                     12874.4553  -0.0028  0.002
  18:  8  2  7     7  2  6                     10366.0428   0.0029  0.002
  19:  7  2  5     6  2  4                      9677.2221   0.0014  0.002
  20:  7  2  6     6  2  5                      9120.5763   0.0003  0.002
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

       10000            A  /MHz         1202.3049(16)                         1
       20000            B  /MHz          724.43428(11)                        2
       30000            C  /MHz          600.80980(12)                        3
         200      DELTA J  /kHz            0.07899(68)                        4
        2000      DELTA K  /kHz           [-0.144453483]                       5
        1100     DELTA JK  /kHz           [ 0.241259522]                       6
       40100      delta J  /kHz           [ 0.013217235]                       7
       41000      delta K  /kHz           [ 0.061912479]                       8

 MICROWAVE AVG =       -0.000067 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001808 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        0.90386         0.90386

  distinct frequency lines in fit:    20
       distinct parameters of fit:     4

                                    upper state  lower state         overall
     limits of quantum number  1:      5   10       4    9           4   10
     limits of quantum number  2:      0    3       0    3           0    3
     limits of quantum number  3:      4   10       3    9           3   10

                 frequency range:        6245        12874

 Standard errors are obtained by muliplying the previous errors by:   1.010546

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000            A  /MHz         1202.3049(17)                         1
       20000            B  /MHz          724.43428(11)                        2
       30000            C  /MHz          600.80981(12)                        3
         200      DELTA J  /kHz            0.07899(68)                        4
        2000      DELTA K  /kHz           [-0.144453483]                       5
        1100     DELTA JK  /kHz           [ 0.241259522]                       6
       40100      delta J  /kHz           [ 0.013217235]                       7
       41000      delta K  /kHz           [ 0.061912479]                       8
```

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DELTA J
A	1.0000			
B	0.1944	1.0000		
C	-0.3167	0.2783	1.0000	
-DELTA J	-0.0529	-0.5175	-0.8719	1.0000

Mean value of |C.ij|, i.ne.j = 0.3719
Mean value of C.ij, i.ne.j = -0.2144

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

10:	-1.6		15:	1.5		18:	1.4		17:	-1.4	
14:	-1.3		1:	0.9		3:	0.8		2:	0.8	
8:	-0.8		9:	-0.7		19:	0.7		16:	-0.6	
4:	-0.6		13:	-0.4		20:	0.1		5:	0.1	
11:	0.1		12:	-0.1		7:	0.1		6:	-0.1	

10:	5	1	5	4	1	4	6245.4937	-0.0032	0.002
15:	8	2	6	7	2	5	11016.6365	0.0031	0.002
18:	8	2	7	7	2	6	10366.0428	0.0029	0.002
17:	10	1	9	9	1	8	12874.4553	-0.0028	0.002
14:	8	3	5	7	3	4	11007.9533	-0.0026	0.002
1:	8	1	8	7	1	7	9881.4978	0.0019	0.002
3:	9	1	9	8	1	8	11085.5815	0.0017	0.002
2:	8	0	8	7	0	7	9892.6754	0.0017	0.002
8:	6	0	6	5	0	5	7505.7448	-0.0016	0.002
9:	5	0	5	4	0	4	6316.3959	-0.0014	0.002

EF-OD:DOH

```
--------------------------------------------------------------------------------
=========
                                                obs         o-c     error     blends
Notes
                                                                              o-c      wt
    / instead of : below denotes (o-c)>3*err
--------------------------------------------------------------------------------
=========
   1:  6  1  6     5  1  5                      7626.3032  -0.0021  0.002
   2:  6  0  6     5  0  5                      7663.9794   0.0011  0.002
   3:  7  0  7     6  0  6                      8883.0570   0.0003  0.002
   4:  7  1  7     6  1  6                      8863.6377   0.0026  0.002
   5:  8  1  8     7  1  7                     10096.7099   0.0018  0.002
   6/  8  0  8     7  0  7                     10106.0637  -0.0064  0.002
   7:  9  1  9     8  1  8                     11327.4147   0.0000  0.002
   8:  9  0  9     8  0  8                     11331.7326   0.0038  0.002
   9: 10  1 10     9  1  9                     12556.9072  -0.0038  0.002
  10: 10  0 10     9  0  9                     12558.8387   0.0026  0.002
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000            A  /MHz         1197.553(26)                          1
        20000            B  /MHz          740.3972(73)                         2
        30000            C  /MHz          614.3054(14)                         3
          200      DELTA J  /kHz            0.0723(38)                         4
         2000      DELTA K  /kHz          [-0.144453483]                       5
         1100     DELTA JK  /kHz          [ 0.241259522]                       6
        40100      delta J  /kHz          [ 0.013217235]                       7
        41000      delta K  /kHz          [ 0.061912479]                       8

 MICROWAVE AVG =       -0.000006 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.003061 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.53066         1.53066

  distinct frequency lines in fit:    10
       distinct parameters of fit:     4

                                    upper state  lower state         overall
     limits of quantum number  1:      6   10       5    9           5   10
     limits of quantum number  2:      0    1       0    1           0    1
     limits of quantum number  3:      6   10       5    9           5   10

                  frequency range:        7626        12558

 Standard errors are obtained by muliplying the previous errors by:   1.976074

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

        10000            A  /MHz         1197.554(51)                          1
        20000            B  /MHz          740.397(14)                          2
        30000            C  /MHz          614.3054(29)                         3
          200      DELTA J  /kHz            0.0723(75)                         4
         2000      DELTA K  /kHz          [-0.144453483]                       5
         1100     DELTA JK  /kHz          [ 0.241259522]                       6
        40100      delta J  /kHz          [ 0.013217235]                       7
        41000      delta K  /kHz          [ 0.061912479]                       8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DELTA J

A           1.0000
B           0.8567   1.0000
C          -0.9503  -0.9653   1.0000
-DELTA J    0.9274   0.9401  -0.9888   1.0000

 Mean value of |C.ij|, i.ne.j =   0.9381
```

Mean value of C.ij, i.ne.j = -0.0300

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

6:	-3.2			8:	1.9			9:	-1.9	10:	1.3
4:	1.3			1:	-1.0			5:	0.9	2:	0.6
3:	0.1			7:	0.0						

6/	8	0	8	7	0	7		10106.0637	-0.0064	0.002
8:	9	0	9	8	0	8		11331.7326	0.0038	0.002
9:	10	1	10	9	1	9		12556.9072	-0.0038	0.002
10:	10	0	10	9	0	9		12558.8387	0.0026	0.002
4:	7	1	7	6	1	6		8863.6377	0.0026	0.002
1:	6	1	6	5	1	5		7626.3032	-0.0021	0.002
5:	8	1	8	7	1	7		10096.7099	0.0018	0.002
2:	6	0	6	5	0	5		7663.9794	0.0011	0.002
3:	7	0	7	6	0	6		8883.0570	0.0003	0.002
7:	9	1	9	8	1	8		11327.4147	0.0000	0.002

/ SPFIT output reformatted with PIFORM

EF-OH:DOH

```
-------------------------------------------------------------------------------
=========
                                                obs         o-c     error     blends
Notes
                                                                              o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------
=========
   1:  7  1  7    6  1  6                      8884.2397   0.0005  0.002
   2:  7  0  7    6  0  6                      8903.7234   0.0008  0.002
   3:  8  1  8    7  1  7                     10119.6178   0.0033  0.002
   4:  8  0  8    7  0  7                     10128.9781   0.0014  0.002
   5:  6  1  6    5  1  5                      7644.5507  -0.0029  0.002
   6:  6  0  6    5  0  5                      7682.4709  -0.0016  0.002
   7:  9  0  9    8  0  8                     11356.9021  -0.0001  0.002
   8:  9  1  9    8  1  8                     11352.6004  -0.0010  0.002
   9: 10  1 10    9  1  9                     12584.3715   0.0015  0.002
  10: 10  0 10    9  0  9                     12586.2845   0.0011  0.002
  11: 11  1 11   10  1 10                     13815.5553  -0.0001  0.002
  12: 11  0 11   10  0 10                     13816.3848  -0.0015  0.002
  13: 12  1 12   11  1 11                     15046.4735  -0.0008  0.002
  14: 12  0 12   11  0 11                     15046.8286   0.0001  0.002
  15:  9  3  7    8  3  6                     12255.6099  -0.0015  0.002
  16:  9  1  8    8  1  7                     11961.6499   0.0002  0.002
  17:  9  2  8    8  2  7                     11875.7462   0.0002  0.002
  18:  8  3  6    7  3  5                     10929.7452   0.0019  0.002
  19:  8  1  7    7  1  6                     10755.9264  -0.0019  0.002
  20:  8  2  7    7  2  6                     10617.5247  -0.0010  0.002
  21:  7  2  5    6  2  4                      9928.8395   0.0022  0.002
  22:  7  1  6    6  1  5                      9539.3617   0.0017  0.002
  23:  7  2  6    6  2  5                      9344.6336   0.0006  0.002
  24:  6  1  5    5  1  4                      8288.7475   0.0002  0.002
  25:  5  2  3    4  2  2                      7076.5849  -0.0019  0.002
  26:  5  1  4    4  1  3                      6988.2680  -0.0018  0.002
  27:  5  1  5    4  1  4                      6397.8600  -0.0012  0.002
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

       10000            A  /MHz         1207.2160(20)                         1
       20000            B  /MHz          744.00294(16)                        2
       30000            C  /MHz          615.44832(11)                        3
         200      DELTA J  /kHz            0.08250(50)                        4
        1100     DELTA JK  /kHz            0.221(14)                          5
        2000      DELTA K  /kHz          [-0.144453483]                       6
       40100      delta J  /kHz          [ 0.013217235]                       7
       41000      delta K  /kHz          [ 0.061912479]                       8

 MICROWAVE AVG =       -0.000062 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001516 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.75821         0.75821

  distinct frequency lines in fit:    27
       distinct parameters of fit:     5

                                  upper state  lower state         overall
      limits of quantum number  1:      5   12       4   11          4   12
      limits of quantum number  2:      0    3       0    3          0    3
      limits of quantum number  3:      3   12       2   11          2   12

                 frequency range:        6397        15046

 Standard errors are obtained by muliplying the previous errors by:   0.839963

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000            A  /MHz         1207.2160(16)                         1
       20000            B  /MHz          744.00295(13)                        2
```

```
        30000            C  /MHz          615.448327(92)                        3
          200      DELTA J  /kHz            0.08250(41)                         4
         1100     DELTA JK  /kHz            0.221(12)                           5
         2000      DELTA K  /kHz          [-0.144453483]                        6
        40100      delta J  /kHz          [ 0.013217235]                        7
        41000      delta K  /kHz          [ 0.061912479]                        8

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DELTA J -DELTA J

A           1.0000
B           0.2735   1.0000
C          -0.5744  -0.1923   1.0000
-DELTA J    0.5561   0.3433  -0.8862   1.0000
-DELTA JK  -0.6205  -0.6992   0.2629  -0.5481   1.0000

 Mean value of |C.ij|, i.ne.j =   0.4956
 Mean value of  C.ij,  i.ne.j =  -0.2085


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

     3:    1.6          5:   -1.4         21:    1.1         19:   -0.9
    18:    0.9         25:   -0.9         26:   -0.9         22:    0.8
     6:   -0.8         15:   -0.8         12:   -0.8          9:    0.8
     4:    0.7         27:   -0.6         10:    0.6         20:   -0.5
     8:   -0.5          2:    0.4         13:   -0.4         23:    0.3
     1:    0.2         24:    0.1         17:    0.1         16:    0.1
    14:    0.1         11:   -0.1          7:   -0.1

     3:  8  1  8    7  1  7                   10119.6178   0.0033  0.002
     5:  6  1  6    5  1  5                    7644.5507  -0.0029  0.002
    21:  7  2  5    6  2  4                    9928.8395   0.0022  0.002
    19:  8  1  7    7  1  6                   10755.9264  -0.0019  0.002
    18:  8  3  6    7  3  5                   10929.7452   0.0019  0.002
    25:  5  2  3    4  2  2                    7076.5849  -0.0019  0.002
    26:  5  1  4    4  1  3                    6988.2680  -0.0018  0.002
    22:  7  1  6    6  1  5                    9539.3617   0.0017  0.002
     6:  6  0  6    5  0  5                    7682.4709  -0.0016  0.002
    15:  9  3  7    8  3  6                   12255.6099  -0.0015  0.002

                                              _____________________________________
_____________________________________________/ SPFIT output reformatted with PIFORM
```

CALCULATED STRUCTURES OF CONFORMERS
(MP2/6-311++G(d,p))

Conf. 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.244931	0.836360	0.217850
2	6	0	1.825550	0.308549	-1.115530
3	6	0	1.777146	-1.239423	-0.966025
4	6	0	1.005157	-1.421670	0.352197
5	6	0	1.639779	-0.292662	1.187094
6	6	0	-0.464010	-0.936173	0.202189
7	6	0	-0.279822	0.623430	0.219653
8	6	0	-1.152969	-1.443147	-1.067871
9	6	0	-1.304099	-1.381429	1.405743
10	6	0	1.660621	2.250966	0.574166
11	8	0	-0.992188	1.354666	-0.782271
12	1	0	1.266934	0.670879	-1.988377
13	1	0	2.852977	0.669146	-1.238977
14	1	0	1.318890	-1.746307	-1.818352
15	1	0	2.789113	-1.643942	-0.852030
16	1	0	1.072927	-2.433004	0.768671
17	1	0	2.726769	-0.398936	1.289376
18	1	0	1.199186	-0.163998	2.181845
19	1	0	-0.680767	1.024693	1.158810
20	1	0	-0.687928	-1.078339	-1.990586
21	1	0	-1.109062	-2.538338	-1.096974
22	1	0	-2.205532	-1.143236	-1.075198
23	1	0	-1.443158	-2.469261	1.391551
24	1	0	-2.289762	-0.904189	1.374212
25	1	0	-0.820447	-1.114518	2.351640
26	1	0	1.283037	2.963235	-0.167849
27	1	0	2.752557	2.338522	0.611310
28	1	0	1.258260	2.538148	1.552821
29	1	0	-0.716992	1.021343	-1.642859
30	1	0	-2.809735	1.176315	-0.362245
31	8	0	-3.668230	0.862661	-0.037325
32	1	0	-4.187633	1.664364	0.053184

Rotational constants (GHz): 1.2258860 0.7617266 0.6300349

Conf. 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.245861	0.824759	0.218302
2	6	0	1.809611	0.307219	-1.124867
3	6	0	1.765998	-1.240440	-0.977146
4	6	0	0.999495	-1.427092	0.343300
5	6	0	1.639087	-0.306710	1.184940
6	6	0	-0.469169	-0.935865	0.195889
7	6	0	-0.279346	0.615700	0.220748
8	6	0	-1.151627	-1.442600	-1.078464
9	6	0	-1.306391	-1.384988	1.400546
10	6	0	1.674660	2.235046	0.583496
11	8	0	-0.969520	1.251243	-0.866412
12	1	0	1.210596	0.665113	-1.968312
13	1	0	2.834828	0.669414	-1.263906
14	1	0	1.300122	-1.742685	-1.827682
15	1	0	2.778177	-1.646739	-0.869094
16	1	0	1.060357	-2.441189	0.754039
17	1	0	2.726262	-0.414825	1.283423
18	1	0	1.200720	-0.183304	2.181531
19	1	0	-0.684859	1.015430	1.163925
20	1	0	-0.729409	-1.005904	-1.985953
21	1	0	-1.050749	-2.533440	-1.133130
22	1	0	-2.219131	-1.203375	-1.055307
23	1	0	-1.455032	-2.471176	1.372075
24	1	0	-2.288268	-0.899493	1.380044
25	1	0	-0.816841	-1.135061	2.348089
26	1	0	1.354210	2.961119	-0.176028
27	1	0	2.766109	2.302739	0.651727
28	1	0	1.249409	2.538683	1.547673
29	1	0	-0.741637	2.187270	-0.821983
30	1	0	-2.813494	1.080527	-0.410844
31	8	0	-3.646769	0.963644	0.070688
32	1	0	-4.320137	1.067617	-0.604954

Rotational constants (GHz): 1.2236414 0.7633667 0.6325645

Conf. 3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.125647	0.017124	-1.018099
2	6	0	-0.472147	1.280613	-0.219412
3	6	0	0.361860	1.290334	1.082875
4	6	0	-0.307693	0.201780	1.969700
5	6	0	-1.353660	-0.409152	1.020257
6	6	0	-1.855508	0.865210	0.314180
7	6	0	-0.656785	-1.171842	-0.140371
8	6	0	-0.385215	2.558124	-1.033843
9	6	0	0.451652	-2.118992	0.323961
10	6	0	-1.689205	-1.987312	-0.928953
11	8	0	1.273337	-0.006675	-1.329852
12	1	0	1.418591	1.085807	0.898972
13	1	0	0.292279	2.280417	1.548382
14	1	0	0.403751	-0.527038	2.363724
15	1	0	-0.819105	0.657859	2.824903
16	1	0	-2.111467	-1.018187	1.526634
17	1	0	-2.584256	0.686280	-0.484210
18	1	0	-2.267591	1.603229	1.013044
19	1	0	-0.683554	0.047747	-1.967414
20	1	0	0.641258	2.725496	-1.378043
21	1	0	-0.691160	3.421485	-0.432187
22	1	0	-1.035503	2.504918	-1.915367
23	1	0	1.306753	-1.600095	0.760325
24	1	0	0.049682	-2.815745	1.069456
25	1	0	0.822875	-2.718364	-0.516664
26	1	0	-1.237276	-2.402360	-1.839075
27	1	0	-2.057740	-2.824396	-0.324424
28	1	0	-2.548871	-1.379142	-1.228643
29	1	0	1.410923	-0.705142	-1.978654
30	8	0	3.597301	-0.314780	0.302216
31	1	0	2.821962	-0.110555	-0.241135
32	1	0	4.097432	0.504101	0.299694

Rotational constants (GHz): 1.0040261 0.8534486 0.6928658

Conf. 4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.109676	0.019668	-1.017238
2	6	0	-0.565622	1.247185	-0.207254
3	6	0	-1.933141	0.717886	0.262719
4	6	0	-1.357578	-0.521173	0.976155
5	6	0	-0.548999	-1.210044	-0.160009
6	6	0	-0.408956	0.163020	1.975584
7	6	0	0.227158	1.294514	1.118554
8	6	0	-0.549525	2.543487	-0.997309
9	6	0	-1.463834	-2.126031	-0.982138
10	6	0	0.630236	-2.043608	0.347142
11	8	0	1.289383	-0.021664	-1.326519
12	1	0	1.299184	1.149909	0.960160
13	1	0	0.093659	2.274464	1.591330
14	1	0	0.329472	-0.511824	2.413491
15	1	0	-0.996818	0.584061	2.799163
16	1	0	-2.083797	-1.197263	1.441664
17	1	0	-2.435188	1.409011	0.950635
18	1	0	-2.609908	0.488978	-0.568542
19	1	0	-0.666221	0.010486	-1.968106
20	1	0	1.393573	-1.440859	0.841957
21	1	0	0.265706	-2.791721	1.061552
22	1	0	1.106386	-2.570496	-0.486546
23	1	0	-1.759388	-3.000615	-0.390696
24	1	0	-0.940043	-2.480596	-1.878129
25	1	0	-2.374039	-1.608601	-1.303144
26	1	0	0.475732	2.829430	-1.266050
27	1	0	-0.969792	3.363719	-0.404886
28	1	0	-1.135844	2.451292	-1.920100
29	1	0	1.453685	0.679177	-1.967301
30	1	0	2.828270	-0.056409	-0.221450
31	8	0	3.600204	0.100710	0.342067
32	1	0	4.088296	-0.723933	0.293391

Rotational constants (GHz): 1.0029890 0.8536878 0.6939238

KRAITCHMAN SUBSTITUTIONS - KRA OUTPUT

Fenchol-hydrate

Parent species (EFOH:DOH)

Planar calculation will be made from I.a and I.b

EFOH:D2O->EFOH:DOH

The parent species:

X, Y, Z =	1207.21600000	744.00295000	615.44832700
eX, eY, eZ =	0.00160000	0.00013000	0.00009200
IX, IY, IZ =	418.63179829	679.27016284	821.15586773
eIX,eIY,eIZ =	0.00055484	0.00011869	0.00012275
PX, PY, PZ =	540.89711614	280.25875159	138.37304670

Mass = 173.27460000

The isotopic species:

X, Y, Z =	1202.30490000	724.43428000	600.80981000
eX, eY, eZ =	0.00170000	0.00011000	0.00012000
IX, IY, IZ =	420.34179932	697.61884404	841.16303793
eIX,eIY,eIZ =	0.00059434	0.00010593	0.00016801
PX, PY, PZ =	559.22004133	281.94299661	138.39880272

Mass change = 1.00627670
Total mass = 174.28087670
M DM/(M+DM) = 1.00046658

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	4.26847 +- 0.00002	1.35260 +- 0.00032	
+Costain err.	4.26847 +- 0.00035	1.35260 +- 0.00115	

	a	b	c
NONPLANAR:	4.26554 +- 0.00005	1.34219 +- 0.00017	0.16503 +- 0.00137
+Costain err.	4.26554 +- 0.00036	1.34219 +- 0.00113	0.16503 +- 0.00919

R= 4.47477 +- 0.00059

DIX,DIY,DIZ =	1.71000104	18.34868120	20.00717020
DPX,DPY,DPZ =	18.32292519	1.68424502	0.02575602
IXY,IXZ,IYZ =	-260.63836455	-402.52406944	-141.88570489

Fenchol-hydrate

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parent species (EFOD:DOH)

Planar calculation will be made from I.a and I.b

EF-OD:D2O->EF-OD:DOH

The parent species:

X, Y, Z =	1197.55400000	740.39700000	614.30540000
eX, eY, eZ =	0.05100000	0.01400000	0.00290000
IX, IY, IZ =	422.00936659	682.57840726	822.68364400
eIX,eIY,eIZ =	0.01797203	0.01290672	0.00388371
PX, PY, PZ =	541.62634233	281.05730167	140.95206493

Mass = 174.28083000

The isotopic species:

X, Y, Z =	1192.78520000	721.01711000	599.76547000
eX, eY, eZ =	0.00280000	0.00021000	0.00012000
IX, IY, IZ =	423.69657588	700.92512090	842.62771080
eIX,eIY,eIZ =	0.00099461	0.00020415	0.00016859
PX, PY, PZ =	559.92812791	282.69958289	140.99699299

Mass change = 1.00627670
Total mass = 175.28710670
M DM/(M+DM) = 1.00049993

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	4.26835 +- 0.00151	1.34354 +- 0.00717	
+Costain err.	4.26835 +- 0.00155	1.34354 +- 0.00725	

	a	b	c	
NONPLANAR:	4.26325 +- 0.00131	1.32521 +- 0.00454	0.21796	+- 0.02727
+Costain err.	4.26325 +- 0.00136	1.32521 +- 0.00468	0.21796	+- 0.02813

R= 4.46979 +- 0.00234

DIX,DIY,DIZ =	1.68720929	18.34671364	19.94406680
DPX,DPY,DPZ =	18.30178558	1.64228122	0.04492807
IXY,IXZ,IYZ =	-260.56904067	-400.67427741	-140.10523674

Fenchol-hydrate

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parent species (FOH:DOH)

Planar calculation will be made from I.a and I.b

EF-OD:DOH->EFOH:DOH

The parent species:

X, Y, Z =	1207.21600000	744.00295000	615.44832700
eX, eY, eZ =	0.00160000	0.00013000	0.00009200
IX, IY, IZ =	418.63179829	679.27016284	821.15586773
eIX,eIY,eIZ =	0.00055484	0.00011869	0.00012275
PX, PY, PZ =	540.89711614	280.25875159	138.37304670

Mass = 173.27460000

The isotopic species:

X, Y, Z =	1197.55400000	740.39700000	614.30540000
eX, eY, eZ =	0.05100000	0.01400000	0.00290000
IX, IY, IZ =	422.00936659	682.57840726	822.68364400
eIX,eIY,eIZ =	0.01797203	0.01290672	0.00388371
PX, PY, PZ =	541.62634233	281.05730167	140.95206493

Mass change = 1.00627670
Total mass = 174.28087670
M DM/(M+DM) = 1.00046658

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.80661 +- 0.00352	1.84901 +- 0.00492	
+Costain err.	1.80661 +- 0.00362	1.84901 +- 0.00499	

	a	b	c	
NONPLANAR:	0.84970 +- 0.00655	0.88649 +- 0.00624	1.61153	+- 0.00351
+Costain err.	0.84970 +- 0.00678	0.88649 +- 0.00646	1.61153	+- 0.00363
			R= 2.02605	+- 0.00494

DIX,DIY,DIZ =	3.37756831	3.30824442	1.52777627
DPX,DPY,DPZ =	0.72922619	0.79855008	2.57901823
IXY,IXZ,IYZ =	-260.63836455	-402.52406944	-141.88570489

Fenchol-hydrate

EF-H...DOD

Planar calculation will be made from I.a and I.b

EF-D...D2O->EF-H...DOD

The parent species:

X, Y, Z =	1202.30490000	724.43428000	600.80981000
eX, eY, eZ =	0.00170000	0.00011000	0.00012000
IX, IY, IZ =	420.34179932	697.61884404	841.16303793
eIX,eIY,eIZ =	0.00059434	0.00010593	0.00016801
PX, PY, PZ =	559.22004133	281.94299661	138.39880272

Mass = 174.28083000

The isotopic species:

X, Y, Z =	1192.78520000	721.01711000	599.76547000
eX, eY, eZ =	0.00280000	0.00021000	0.00012000
IX, IY, IZ =	423.69657588	700.92512090	842.62771080
eIX,eIY,eIZ =	0.00099461	0.00020415	0.00016859
PX, PY, PZ =	559.92812791	282.69958289	140.99699299

Mass change = 1.00627670
Total mass = 175.28710670
M DM/(M+DM) = 1.00049993

KRAITCHMAN RESULTS:

	a	b
PLANAR:	1.80683 +- 0.00006	1.84203 +- 0.00032
+Costain err.	1.80683 +- 0.00083	1.84203 +- 0.00087

	a	b	c
NONPLANAR:	0.83752 +- 0.00036	0.86280 +- 0.00034	1.61709 +- 0.00019
+Costain err.	0.83752 +- 0.00183	0.86280 +- 0.00177	1.61709 +- 0.00095

R= 2.01515 +- 0.00131

DIX,DIY,DIZ =	3.35477656	3.30627686	1.46467286
DPX,DPY,DPZ =	0.70808658	0.75658628	2.59819028
IXY,IXZ,IYZ =	-277.27704472	-420.82123861	-143.54419389

Fenchol-hydrate

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parent species EFD...HOD

Planar calculation will be made from I.a and I.b

EF-D...D2O->EF-D...HOD

The parent species:

X, Y, Z =	1195.99600000	729.32010000	606.17140000
eX, eY, eZ =	0.02800000	0.00450000	0.00840000
IX, IY, IZ =	422.55910973	692.94539531	833.72294536
eIX,eIY,eIZ =	0.00989272	0.00427556	0.01155329
PX, PY, PZ =	552.05461547	281.66832989	140.89077984

Mass = 174.28083000

The isotopic species:

X, Y, Z =	1192.78520000	721.01711000	599.76547000
eX, eY, eZ =	0.00280000	0.00021000	0.00012000
IX, IY, IZ =	423.69657588	700.92512090	842.62771080
eIX,eIY,eIZ =	0.00099461	0.00020415	0.00016859
PX, PY, PZ =	559.92812791	282.69958289	140.99699299

Mass change = 1.00627670
Total mass = 175.28710670
M DM/(M+DM) = 1.00049993

KRAITCHMAN RESULTS:

	a	b
PLANAR:	2.81819 +- 0.00076	1.08187 +- 0.00473
+Costain err.	2.81819 +- 0.00093	1.08187 +- 0.00493

	a	b	c
NONPLANAR:	2.79956 +- 0.00141	1.02954 +- 0.00395	0.33013 +- 0.01230
+Costain err.	2.79956 +- 0.00151	1.02954 +- 0.00421	0.33013 +- 0.01312

R= 3.00108 +- 0.00248

DIX,DIY,DIZ =	1.13746615	7.97972560	8.90476544
DPX,DPY,DPZ =	7.87351244	1.03125300	0.10621315
IXY,IXZ,IYZ =	-270.38628558	-411.16383563	-140.77755005
