Fits of Spectroscopic Parameters

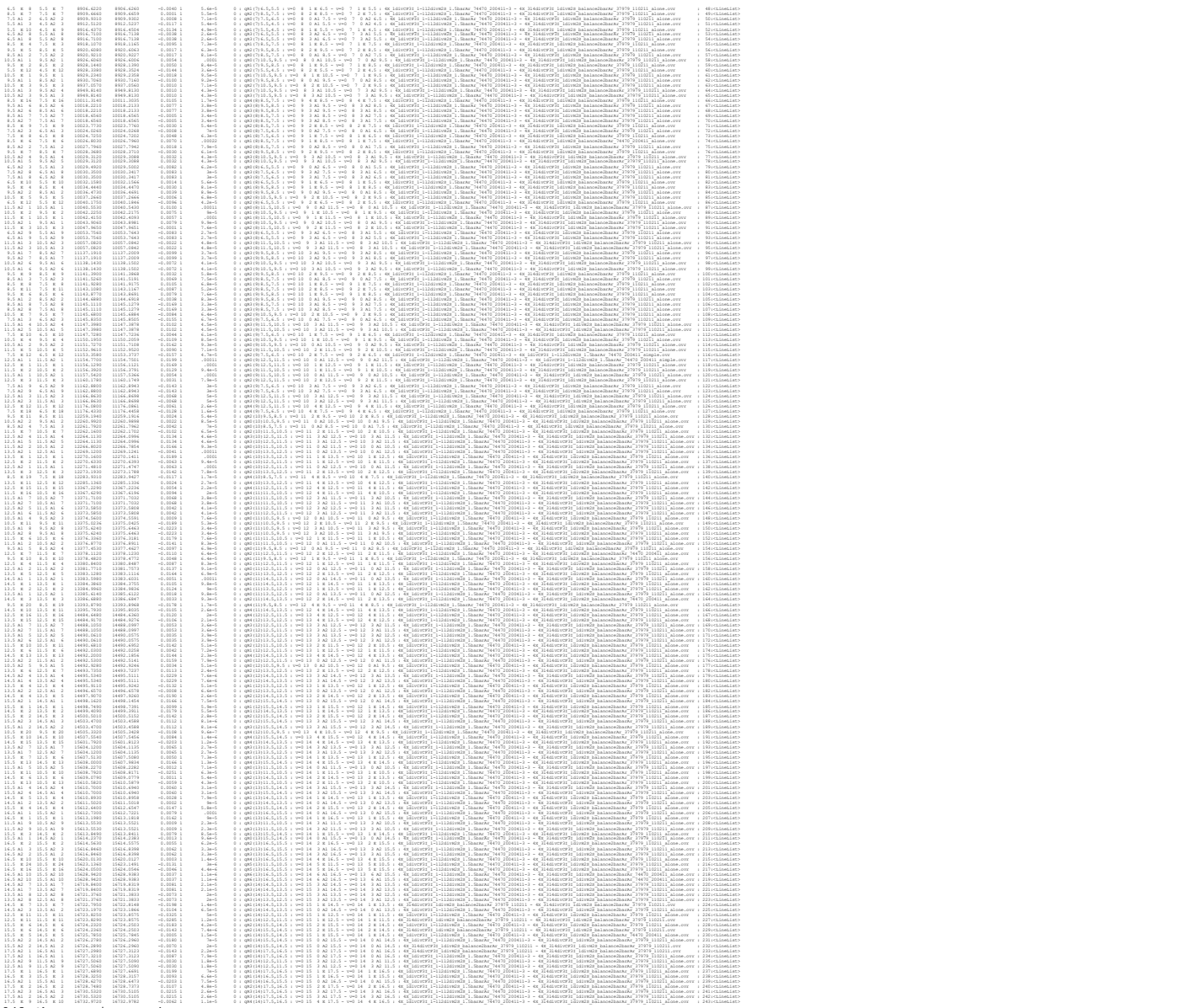
The results of the spectroscopic fits performed in PGOPHER (the .log files output by the program) are provided below. The small font size used to display individual transitions and the associated residuals allows the lists to be displayed in a convenient format (it avoids wrapping over multiple lines) but it will be necessary to use the zoom function in either Microsoft Word or Adobe Acrobat to view.

The original .log files of each individual fit are also available from the corresponding authors on request.

$H_2S \cdots ICF_3$

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_H2S_su_060511_2.pgo
  Units                 MHz
  PrintLevel            Detail
  Precision             4
  BasisOrder            boDefault
  QuantumNumberFormat J
  FitCycles             1
  FitDetails            False
  AutoReplot            True
  AllowComplex          False
  NoLineList            False
  ShowEstUnc            False
  ShowDerivatives       False
  SVDThresh     1E-15
  ScaleChanges 1
  Species: Species
    Jmax 60
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei          1
      JAdjustSym       False
      BlockMatrix      True
      PointGroup       C3v
      AlternateBasis False
      wt(A1,A2)        1
      wt(E)            1
      (Wt2)            1
      (Wt3)            1
      (Wt4)            1
      (Wt5)            1
      (Wt6)            1
      (Wt7)            1
      (Wt8)            1
      (Wt9)            1
      (Wt10)           1
      (Wt11)           1
      (Wt12)           1
      (Wt13)           1
      Abundance 1
      SymmetricManifold: Ground
        Initial         True
        EigenSearch     True
        LimitSearch     False
        AutoQConverge True
        UsePopParams    False
        SymmetricTop: v=0
          Symmetry A1
          Kmin      all
          Kmax      all
          B    557.574730880983           Float
          C    5600
          DJ   0.000124483669799597       Float
          DJK  0.00272495699858938        Float
          symmetricTopNucleus: Nucleus1
            Spin    2.5
            AsNext False
            eQq -2166.54541764924            Float
        <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
        <J,N,K,l|C|J,N,K,l> = K^2
        <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
        <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
      TransitionMoments: <Ground|mu|Ground>
        CartesianTransitionMoment: <v=0|a|v=0>
          Axis a
          Strength 1
```

```
Residuals before fit for SymmetricTop for the Ground manifold
   J' S' #'    J" S" #"     Observed    Calculated     Obs-Calc  StdDev
  4.5 A1  3   3.5 A2  3    6660.7520    6660.7633     -0.0113 1       9e-5     0 : qR0(5)4.5,3.5 : v=0  6  0 A1 4.5 - v=0  5  0 A2 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  1:<LineList>
  4.5  E  7   3.5  E  5    6665.3710    6665.3774     -0.0064 1     7.8e-5     0 : qR1(5)4.5,3.5 : v=0  6  1 E 4.5 - v=0  5  1 E 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  2:<LineList>
  5.5  E  5   4.5  E  4    6666.3420    6666.3373      0.0047 1     9.5e-5     0 : qR1(5)5.5,4.5 : v=0  6  1 E 5.5 - v=0  5  1 E 4.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  3:<LineList>
  3.5 A1  3   2.5 A2  3    6674.5450    6674.5464     -0.0014 1     7.4e-5     0 : qR0(5)3.5,2.5 : v=0  6  0 A1 3.5 - v=0  5  0 A2 2.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  4:<LineList>
  6.5  E  3   5.5  E  3    6681.2540    6681.2519      0.0021 1     .00035     0 : qR1(5)6.5,5.5 : v=0  6  1 E 6.5 - v=0  5  1 E 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  5:<LineList>
  3.5  E  8   2.5  E  5    6684.9450    6684.9558     -0.0108 1     .00019     0 : qR1(5)3.5,2.5 : v=0  6  1 E 3.5 - v=0  5  1 E 2.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  6:<LineList>
  6.5 A1  2   5.5 A2  2    6687.2180    6687.2249     -0.0069 1     .00046     0 : qR0(5)6.5,5.5 : v=0  6  0 A1 6.5 - v=0  5  0 A2 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  7:<LineList>
  7.5  E  2   6.5  E  2    6699.4370    6699.4279      0.0091 1     .00042     0 : qR1(5)7.5,6.5 : v=0  6  1 E 7.5 - v=0  5  1 E 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  8:<LineList>
  8.5 A1  1   7.5 A2  1    6700.2920    6700.2849      0.0071 1     .00065     0 : qR0(5)8.5,7.5 : v=0  6  0 A1 8.5 - v=0  5  0 A2 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   :  9:<LineList>
  8.5  E  1   7.5  E  1    6706.2740    6706.2721      0.0019 1      .0005     0 : qR1(5)8.5,7.5 : v=0  6  1 E 8.5 - v=0  5  1 E 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 10:<LineList>
  7.5 A1  1   6.5 A2  1    6706.9530    6706.9459      0.0071 1     .00055     0 : qR0(5)7.5,6.5 : v=0  6  0 A1 7.5 - v=0  5  0 A2 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 11:<LineList>
  7.5 A2  6   6.5 A1  6    7767.8830    7767.8786      0.0044 1     4.2e-5     0 : qR3(6)7.5,6.5 : v=0  7  3 A2 7.5 - v=0  6  3 A1 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 12:<LineList>
  7.5 A1  6   6.5 A2  6    7767.8830    7767.8786      0.0044 1     4.2e-5     0 : qR3(6)7.5,6.5 : v=0  7  3 A1 7.5 - v=0  6  3 A2 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 13:<LineList>
  6.5 A2  7   5.5 A1  7    7777.4560    7777.4525      0.0035 1     3.6e-5     0 : qR3(6)6.5,5.5 : v=0  7  3 A2 6.5 - v=0  6  3 A1 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 14:<LineList>
  6.5 A1  7   5.5 A2  7    7777.4560    7777.4525      0.0035 1     3.6e-5     0 : qR3(6)6.5,5.5 : v=0  7  3 A1 6.5 - v=0  6  3 A2 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 15:<LineList>
  8.5 A1  5   7.5 A2  5    7783.0550    7783.0480      0.0070 1     4.9e-5     0 : qR3(6)8.5,7.5 : v=0  7  3 A1 8.5 - v=0  6  3 A2 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 16:<LineList>
  8.5 A2  5   7.5 A1  5    7783.0550    7783.0480      0.0070 1     4.9e-5     0 : qR3(6)8.5,7.5 : v=0  7  3 A2 8.5 - v=0  6  3 A1 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 17:<LineList>
  6.5  E  9   5.5  E  9    7784.7680    7784.7786     -0.0106 1     .00013     0 : qR2(6)6.5,5.5 : v=0  7  2 E 6.5 - v=0  6  2 E 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 18:<LineList>
  5.5 A2  3   4.5 A1  3    7784.8430    7784.8428      0.0002 1     .00033     0 : qR0(6)5.5,4.5 : v=0  7  0 A2 5.5 - v=0  6  0 A1 4.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 19:<LineList>
  5.5  E  7   4.5  E  7    7787.1360    7787.1363     -0.0003 1     .00025     0 : qR1(6)5.5,4.5 : v=0  7  1 E 5.5 - v=0  6  1 E 4.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 20:<LineList>
  7.5  E  7   6.5  E  7    7788.5320    7788.5354     -0.0034 1     .00016     0 : qR2(6)7.5,6.5 : v=0  7  2 E 7.5 - v=0  6  2 E 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 21:<LineList>
  6.5  E  5   5.5  E  5    7789.0010    7789.0061     -0.0051 1      .0003     0 : qR1(6)6.5,5.5 : v=0  7  1 E 6.5 - v=0  6  1 E 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 22:<LineList>
  6.5 A2  2   5.5 A1  2    7790.3860    7790.3885     -0.0025 1     .00039     0 : qR0(6)6.5,5.5 : v=0  7  0 A2 6.5 - v=0  6  0 A1 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 23:<LineList>
  5.5  E 11   4.5  E 11    7794.1320    7794.1422     -0.0102 1     .00011     0 : qR2(6)5.5,4.5 : v=0  7  2 E 5.5 - v=0  6  2 E 4.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 24:<LineList>
  4.5 A2  3   3.5 A1  3    7794.4960    7794.5000     -0.0040 1     .00028     0 : qR0(6)4.5,3.5 : v=0  7  0 A2 4.5 - v=0  6  0 A1 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 25:<LineList>
  4.5  E  9   3.5  E  8    7800.6400    7800.6416     -0.0016 1     .00021     0 : qR1(6)4.5,3.5 : v=0  7  1 E 4.5 - v=0  6  1 E 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 26:<LineList>
  7.5  E  3   6.5  E  3    7800.7300    7800.7319     -0.0019 1     .00035     0 : qR1(6)7.5,6.5 : v=0  7  1 E 7.5 - v=0  6  1 E 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 27:<LineList>
  8.5  E  5   7.5  E  5    7801.8420    7801.8451     -0.0031 1     .00018     0 : qR2(6)8.5,7.5 : v=0  7  2 E 8.5 - v=0  6  2 E 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 28:<LineList>
  7.5 A2  2   6.5 A1  2    7804.7540    7804.7620     -0.0080 1     .00045     0 : qR0(6)7.5,6.5 : v=0  7  0 A2 7.5 - v=0  6  0 A1 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 29:<LineList>
  5.5 A1  8   4.5 A2  7    7806.2550    7806.2581     -0.0031 1       3e-5     0 : qR3(6)5.5,4.5 : v=0  7  3 A1 5.5 - v=0  6  3 A2 4.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 30:<LineList>
  5.5 A2  8   4.5 A1  7    7806.2550    7806.2581     -0.0031 1       3e-5     0 : qR3(6)5.5,4.5 : v=0  7  3 A2 5.5 - v=0  6  3 A1 4.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 31:<LineList>
  9.5 A2  1   8.5 A1  1    7813.0930    7813.0853      0.0077 1     9.4e-5     0 : qR0(6)9.5,8.5 : v=0  7  0 A2 9.5 - v=0  6  0 A1 8.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 32:<LineList>
  8.5  E  2   7.5  E  2    7814.0320    7814.0268      0.0052 1     7.4e-5     0 : qR1(6)8.5,7.5 : v=0  7  1 E 8.5 - v=0  6  1 E 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 33:<LineList>
  9.5  E  1   8.5  E  1    7816.9510    7816.9553     -0.0043 1     8.5e-5     0 : qR1(6)9.5,8.5 : v=0  7  1 E 9.5 - v=0  6  1 E 8.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 34:<LineList>
  8.5 A2  1   7.5 A1  1    7818.2550    7818.2485      0.0065 1     8.1e-5     0 : qR0(6)8.5,7.5 : v=0  7  0 A2 8.5 - v=0  6  0 A1 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 35:<LineList>
  4.5  E 12   3.5  E 11    7819.3420    7819.3465     -0.0045 1     2.9e-5     0 : qR2(6)4.5,3.5 : v=0  7  2 E 4.5 - v=0  6  2 E 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 36:<LineList>
  9.5  E  3   8.5  E  3    7828.3770    7828.3806     -0.0036 1     6.2e-5     0 : qR2(6)9.5,8.5 : v=0  7  2 E 9.5 - v=0  6  2 E 8.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 37:<LineList>
  9.5 A1  3   8.5 A2  3    7846.8320    7846.8329     -0.0009 1     3.7e-5     0 : qR3(6)9.5,8.5 : v=0  7  3 A1 9.5 - v=0  6  3 A2 8.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 38:<LineList>
  9.5 A2  4   8.5 A1  4    7846.8320    7846.8329     -0.0009 1     3.7e-5     0 : qR3(6)9.5,8.5 : v=0  7  3 A2 9.5 - v=0  6  3 A1 8.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 39:<LineList>
  4.5 A2  8   3.5 A1  7    7851.4880    7851.4897     -0.0017 1     1.7e-5     0 : qR3(6)4.5,3.5 : v=0  7  3 A2 4.5 - v=0  6  3 A1 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411_simple.ovr   : 40:<LineList>
  4.5 A1  8   3.5 A2  7    7851.4880    7851.4897     -0.0017 1     1.7e-5     0 : qR3(6)4.5,3.5 : v=0  7  3 A1 4.5 - v=0  6  3 A2 3.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411_simple.ovr   : 41:<LineList>
  8.5 A2  6   7.5 A1  6    8895.4820    8895.4822     -0.0002 1     3.4e-5     0 : qR3(7)8.5,7.5 : v=0  8  3 A2 8.5 - v=0  7  3 A1 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 42:<LineList>
  8.5 A1  6   7.5 A2  6    8895.4820    8895.4822     -0.0002 1     3.4e-5     0 : qR3(7)8.5,7.5 : v=0  8  3 A1 8.5 - v=0  7  3 A2 7.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 43:<LineList>
  7.5 A2  7   6.5 A1  7    8898.8330    8898.8332     -0.0002 1     2.9e-5     0 : qR3(7)7.5,6.5 : v=0  8  3 A2 7.5 - v=0  7  3 A1 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 44:<LineList>
  7.5 A1  7   6.5 A2  7    8898.8330    8898.8332     -0.0002 1     2.9e-5     0 : qR3(7)7.5,6.5 : v=0  8  3 A1 7.5 - v=0  7  3 A2 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 45:<LineList>
  7.5  E  9   6.5  E  9    8905.0680    8905.0763     -0.0083 1     4.8e-5     0 : qR2(7)7.5,6.5 : v=0  8  2 E 7.5 - v=0  7  2 E 6.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 46:<LineList>
  6.5 A1  3   5.5 A2  3    8905.3920    8905.3943     -0.0023 1     6.1e-5     0 : qR0(7)6.5,5.5 : v=0  8  0 A1 6.5 - v=0  7  0 A2 5.5 : 4X_1divCF3I_1-112divH2S_1.5barAr_74470_200411-3 - 4X_314divCF3I_1divH2S_balance2barAr_37979_110211_alone.ovr   : 47:<LineList>
```

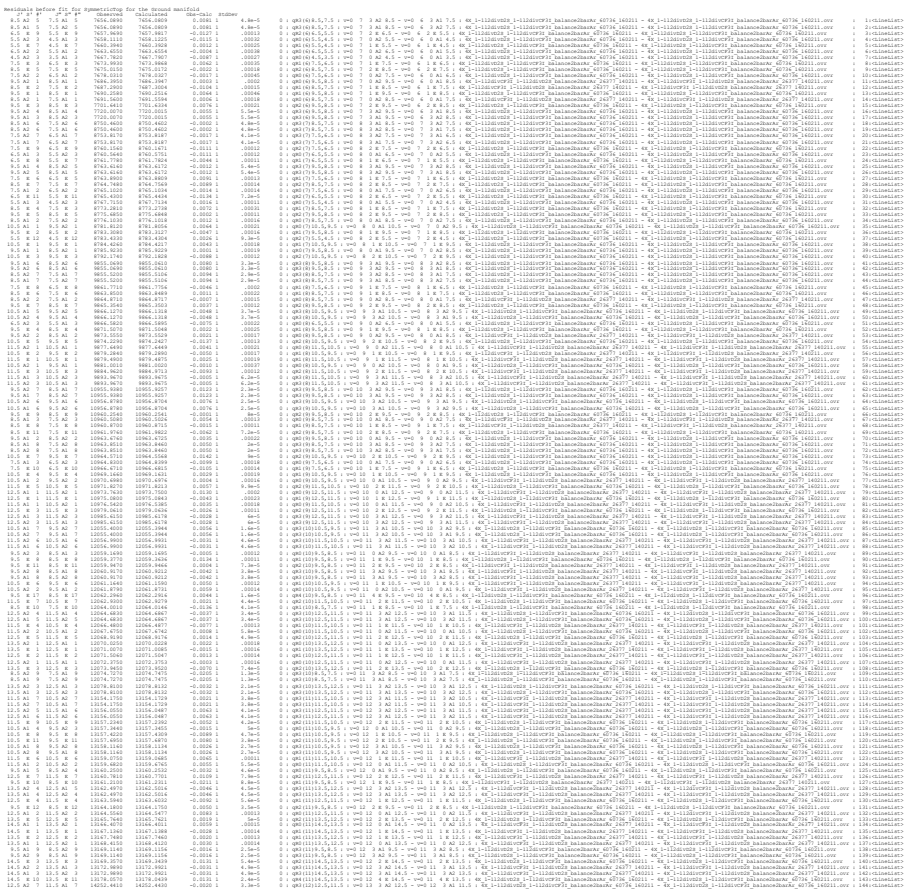


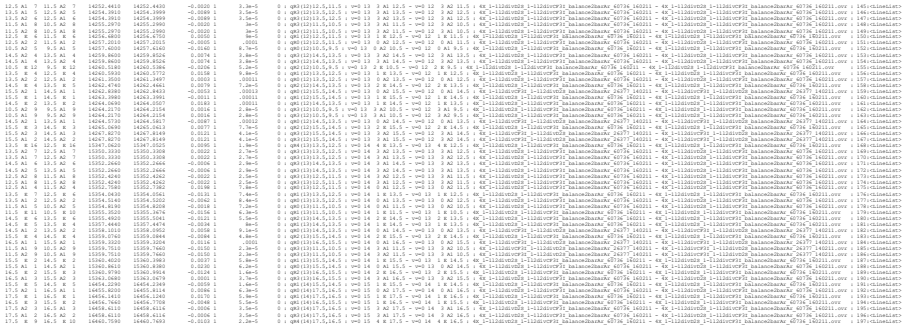
```
243 Observations,  4 Parameters
Initial Average Error: 0.0101814454995942
Predicted New Error:   0.0101814454995936
Parameters:
  # Old                  New                  Std Dev   Change/Std Sens    Summary                Name
  1 557.574730880983     557.5747308814       8.6566e-5    0.0000  1.16e-5 557.574731(87)         v=0 B
  2 .00012448366979597 .00012448367120977 2.6338e-7    0.0000  3.59e-8 1.2448(26)e-4          v=0 DJ
  3 .00272495699858938 .00272495699737624 4.6709e-6    0.0000  1.32e-6 2.7250(47)e-3          v=0 DJK
  4 -2166.54541764924   -2166.54541772604   .11264532    0.0000  .042894 -2166.55(11)           Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.883   1.000
  3   0.227  -0.103   1.000
  4  -0.163  -0.113  -0.167   1.000
```

$HDS\cdots ICF_3$

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_HDS_su_270511.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat  J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
```

```
ShowDerivatives     False
SVDThresh    1E-15
ScaleChanges 1
Species: Species
  Jmax 60
  Concentration 1
  SymmetricMolecule: SymmetricTop
    nNuclei         1
    JAdjustSym      False
    BlockMatrix     True
    PointGroup      C3v
    AlternateBasis False
    wt(A1,A2)       1
    wt(E)           1
    (Wt2)           1
    (Wt3)           1
    (Wt4)           1
    (Wt5)           1
    (Wt6)           1
    (Wt7)           1
    (Wt8)           1
    (Wt9)           1
    (Wt10)          1
    (Wt11)          1
    (Wt12)          1
    (Wt13)          1
    Abundance 1
    SymmetricManifold: Ground
      Initial       True
      EigenSearch   True
      LimitSearch   False
      AutoQConverge True
      UsePopParams  False
      SymmetricTop: v=0
        Symmetry A1
        Kmin      all
        Kmax      all
        B    548.5241532311              Float
        C    5600
        DJ   0.00012350199051638383      Float
        DJK 0.00421389208467024          Float
        symmetricTopNucleus: Nucleus1
          Spin    2.5
          AsNext False
          eQq -2167.01334117607              Float
      <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
      <J,N,K,l|C|J,N,K,l> = K^2
      <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
      <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
    TransitionMoments: <Ground|mu|Ground>
      CartesianTransitionMoment: <v=0|a|v=0>
        Axis a
        Strength 1
```





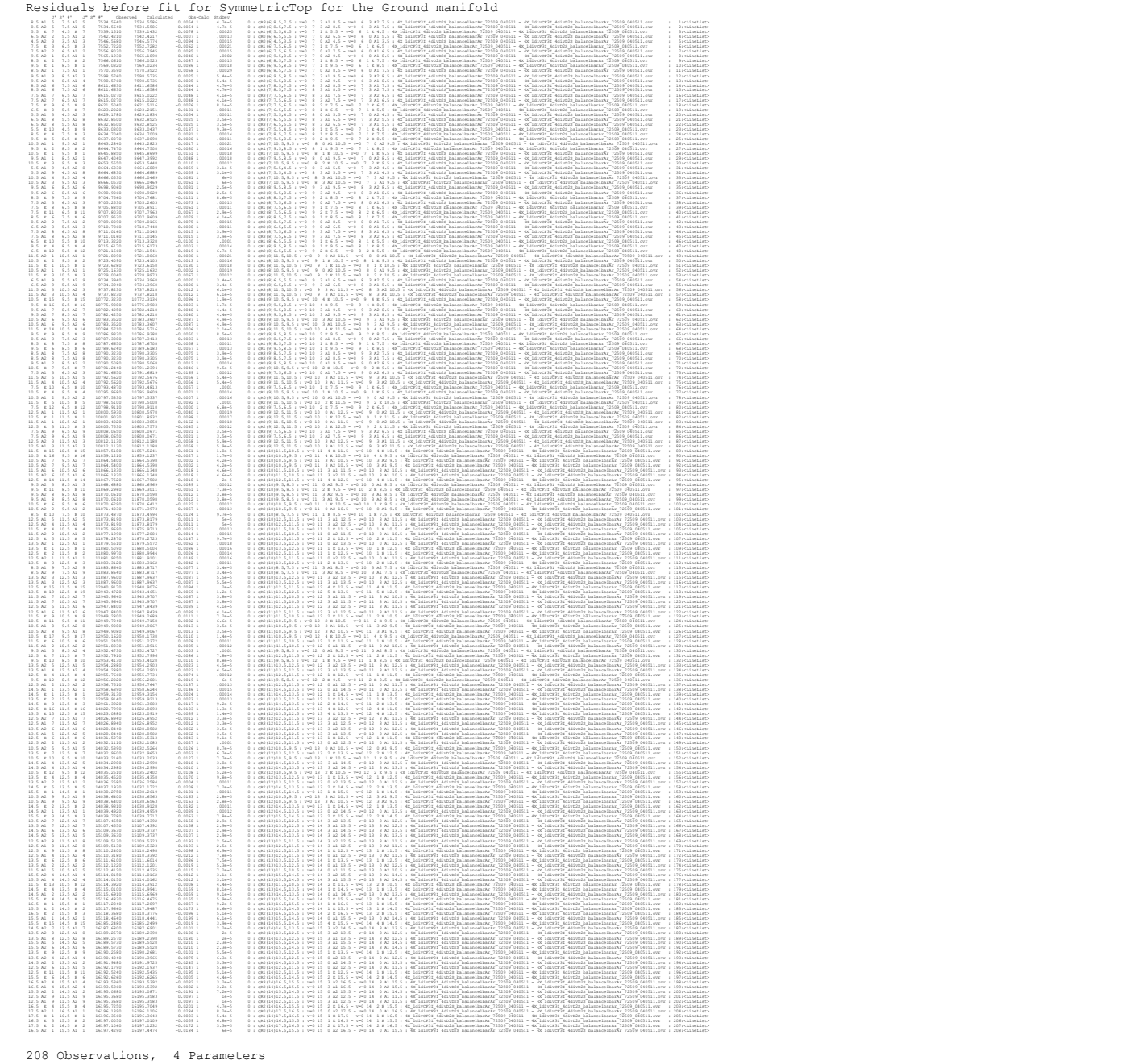
```
197 Observations,  4 Parameters
Initial Average Error: 0.00786487322524606
Predicted New Error:   0.00786487322513152
Parameters:
  # Old                  New                  Std Dev    Change/Std Sens    Summary              Name
  1 548.5241532311       548.524153230871     8.4045e-5    0.0000  8.85e-6 548.524153(84)       v=0 B
  2 .000123501990516383 .000123501989870609 2.7048e-7    0.0000  2.93e-8 1.2350(27)e-4        v=0 DJ
  3 .00421389208467024   .00421389207573259  5.8773e-6    0.0000  1.38e-6 4.2139(59)e-3        v=0 DJK
  4 -2167.01334117607    -2167.0133324603    .11820165    0.0001  .040596 -2167.01(12)         Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.894   1.000
  3   0.240  -0.101   1.000
  4  -0.187  -0.173   0.021   1.000
```

$D_2S\cdots ICF_3$

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_D2S_su_050511.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 60
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei        1
      JAdjustSym     False
      BlockMatrix    True
      PointGroup     C3v
      AlternateBasis False
      wt(A1,A2)      1
      wt(E)          1
      (Wt2)          1
      (Wt3)          1
      (Wt4)          1
      (Wt5)          1
      (Wt6)          1
      (Wt7)          1
      (Wt8)          1
      (Wt9)          1
      (Wt10)         1
      (Wt11)         1
      (Wt12)         1
      (Wt13)         1
      Abundance 1
      SymmetricManifold: Ground
        Initial        True
        EigenSearch    True
        LimitSearch    False
        AutoQConverge True
        UsePopParams   False
        SymmetricTop: v=0
          Symmetry A1
          Kmin     all
          Kmax     all
          B    539.865332937955            Float
          C    5600
          DJ  0.000118928784573447         Float
          DJK 0.00618267163447944          Float
          symmetricTopNucleus: Nucleus1
            Spin   2.5
            AsNext False
            eQq -2166.43501578477            Float
        <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
        <J,N,K,l|C|J,N,K,l> = K^2
        <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
        <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
      TransitionMoments: <Ground|mu|Ground>
        CartesianTransitionMoment: <v=0|a|v=0>
```

```
         Axis a
         Strength 1
```

Residuals before fit for SymmetricTop for the Ground manifold



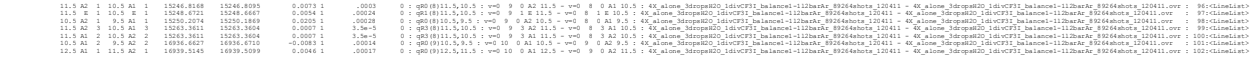
```
208 Observations,  4 Parameters
Initial Average Error: 0.00949105879508888
Predicted New Error:   0.00945023523485998
Parameters:
  # Old                  New                  Std Dev   Change/Std Sens    Summary              Name
  1 539.865332937955     539.865332910769     9.4094e-5   -0.0003  1.03e-5 539.865333(94)        v=0 B
  2 .000118928784573447 .000118928708058664 2.7276e-7   -0.0003  3.17e-9 1.1893(27)e-4        v=0 DJ
  3 .006182671634479 44  .006182670877941    5.9884e-6   -0.0001  1.63e-7 6.1827(60)e-3         v=0 DJK
  4 -2166.43501578477    -2166.53298063685    2.4509018   -0.0400   .026375 -2166.5(25)          Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.894   1.000
  3   0.352   0.029   1.000
  4   0.949   0.921   0.415   1.000
```

$H_2{}^{16}O\cdots ICF_3$, Symmetric top, m=0 transitions.

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_H2O_m=0_species_only.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
```

```
QuantumNumberFormat J
FitCycles           1
FitDetails          False
AutoReplot          True
AllowComplex        False
NoLineList          False
ShowEstUnc          False
ShowDerivatives     False
SVDThresh    1E-15
ScaleChanges 1
Species: Species
  Jmax 30
  Concentration 1
  SymmetricMolecule: SymmetricTop
    nNuclei         1
    JAdjustSym      False
    BlockMatrix     True
    PointGroup      C3v
    AlternateBasis False
    wt(A1,A2)       1
    wt(E)           1
    (Wt2)           1
    (Wt3)           1
    (Wt4)           1
    (Wt5)           1
    (Wt6)           1
    (Wt7)           1
    (Wt8)           1
    (Wt9)           1
    (Wt10)          1
    (Wt11)          1
    (Wt12)          1
    (Wt13)          1
    Abundance 1
    SymmetricManifold: Ground
      Initial       True
      Colour        Green
      EigenSearch   True
      LimitSearch   False
      AutoQConverge True
      UsePopParams  False
      SymmetricTop: v=0
        Symmetry A1
        Kmin     all
        Kmax     all
        B    846.820303741271           Float
        C    5600
        DJ   0.000143068644503587       Float
        DJK  0.00192085550456349        Float
        symmetricTopNucleus: Nucleus1
          Spin    2.5
          AsNext False
          eQq -2199.27458373478           Float
      <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
      <J,N,K,l|C|J,N,K,l> = K^2
      <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
      <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
    TransitionMoments: <Ground|mu|Ground>
      CartesianTransitionMoment: <v=0|a|v=0>
        Axis a
        Strength 1
```

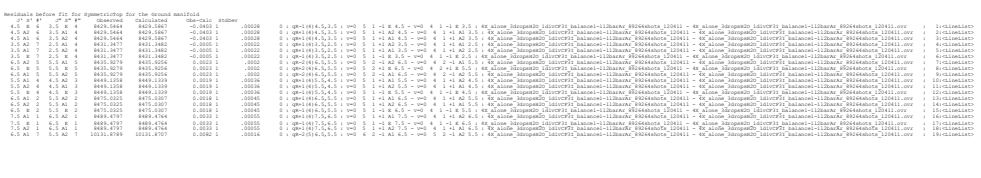
```
Residuals before fit for SymmetricTop for the Ground manifold
   J' S' #'    J" S" #"     Observed    Calculated      Obs-Calc  StdDev
  2.5 A2  3   1.5 A1  2    8442.3750    8442.3835     -0.0085 1       .00018      0 : qR0(4)2.5,1.5 : Ground v=0  5  0 A2 2.5 - Ground v=0  4  0 A1 1.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  1:<LineList>
  3.5 A2  3   2.5 A1  3    8421.0700    8421.0667      0.0033 1       .00023      0 : qR0(4)3.5,2.5 : Ground v=0  5  0 A2 3.5 - Ground v=0  4  0 A1 2.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  2:<LineList>
  4.5 A1  3   3.5 A2  3   10131.4020   10131.3898      0.0122 1       .00025      0 : qR0(5)4.5,3.5 : Ground v=0  6  0 A1 4.5 - Ground v=0  5  0 A2 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  3:<LineList>
  4.5 A2  2   3.5 A1  2    8430.7940    8430.7889      0.0051 1        .0003      0 : qR0(4)4.5,3.5 : Ground v=0  5  0 A2 4.5 - Ground v=0  4  0 A1 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  4:<LineList>
  4.5 A2  3   3.5 A1  3   11843.7360   11843.7429     -0.0069 1       .00018      0 : qR0(6)4.5,3.5 : Ground v=0  7  0 A2 4.5 - Ground v=0  6  0 A1 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  5:<LineList>
  5.5 A2  3   4.5 A1  3   11834.1160   11834.1227     -0.0067 1       .00022      0 : qR0(6)5.5,4.5 : Ground v=0  7  0 A2 5.5 - Ground v=0  6  0 A1 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  6:<LineList>
  5.5 A1  2   4.5 A2  2   10138.8740   10138.8678      0.0062 1        .0003      0 : qR0(5)5.5,4.5 : Ground v=0  6  0 A1 5.5 - Ground v=0  5  0 A2 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  7:<LineList>
  5.5 A1  5   4.5 A2  3   13540.3150   13540.3138      0.0012 1       .00014      0 : qR0(7)5.5,4.5 : Ground v=0  8  0 A1 5.5 - Ground v=0  7  0 A2 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  8:<LineList>
  6.5 A1  4   5.5 A2  3   13533.2220   13533.2278     -0.0058 1       .00016      0 : qR0(7)6.5,5.5 : Ground v=0  8  0 A1 6.5 - Ground v=0  7  0 A2 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   :  9:<LineList>
  6.5 A2  1   5.5 A1  1    8489.9320    8489.9305      0.0015 1       .00048      0 : qR0(4)6.5,5.5 : Ground v=0  5  0 A2 6.5 - Ground v=0  4  0 A1 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 10:<LineList>
  6.5 A1  2   5.5 A2  2   10158.8660   10158.8693     -0.0033 1       .00037      0 : qR0(5)6.5,5.5 : Ground v=0  6  0 A1 6.5 - Ground v=0  5  0 A2 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 11:<LineList>
  6.5 A1  1   5.5 A2  1    6792.9830    6792.9806      0.0024 1       .00058      0 : qR0(3)6.5,5.5 : Ground v=0  4  0 A1 6.5 - Ground v=0  3  0 A2 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 12:<LineList>
  6.5 A2  2   5.5 A1  2   11840.0340   11840.0339      0.0001 1       .00026      0 : qR0(6)6.5,5.5 : Ground v=0  7  0 A2 6.5 - Ground v=0  6  0 A1 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 13:<LineList>
  7.5 A2  1   6.5 A1  1    8480.8120    8480.8026      0.0094 1       .00059      0 : qR0(4)7.5,6.5 : Ground v=0  5  0 A2 7.5 - Ground v=0  4  0 A1 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 14:<LineList>
  7.5 A1  2   6.5 A2  2   13538.0120   13538.0038      0.0082 1       .00019      0 : qR0(7)7.5,6.5 : Ground v=0  8  0 A1 7.5 - Ground v=0  7  0 A2 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 15:<LineList>
  7.5 A2  2   6.5 A1  2   11854.5860   11854.5942     -0.0082 1        .0003      0 : qR0(6)7.5,6.5 : Ground v=0  7  0 A2 7.5 - Ground v=0  6  0 A1 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 16:<LineList>
  7.5 A1  1   6.5 A2  1   10177.7380   10177.7348      0.0032 1       .00044      0 : qR0(5)7.5,6.5 : Ground v=0  6  0 A1 7.5 - Ground v=0  5  0 A2 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 17:<LineList>
  8.5 A1  1   7.5 A2  1   10170.9550   10170.9550      0.0000 1       .00051      0 : qR0(5)8.5,7.5 : Ground v=0  6  0 A1 8.5 - Ground v=0  5  0 A2 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 18:<LineList>
  8.5 A1  2   7.5 A2  2   13549.0800   13549.0790      0.0010 1       .00022      0 : qR0(7)8.5,7.5 : Ground v=0  8  0 A1 8.5 - Ground v=0  7  0 A2 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 19:<LineList>
  8.5 A2  1   7.5 A1  1   11867.5500   11867.5456      0.0044 1       .00035      0 : qR0(6)8.5,7.5 : Ground v=0  7  0 A2 8.5 - Ground v=0  6  0 A1 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 20:<LineList>
  9.5 A1  3   8.5 A2  2   16929.6480   16929.6408      0.0072 1       7.2e-5      0 : qR0(9)9.5,8.5 : Ground v=0 10  0 A1 9.5 - Ground v=0  9  0 A2 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 21:<LineList>
  9.5 A2  1   8.5 A1  1   11862.3160   11862.3164     -0.0004 1        .0004      0 : qR0(6)9.5,8.5 : Ground v=0  7  0 A2 9.5 - Ground v=0  6  0 A1 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 22:<LineList>
  9.5 A1  1   8.5 A2  1   13558.5090   13558.5131     -0.0041 1       .00025      0 : qR0(7)9.5,8.5 : Ground v=0  8  0 A1 9.5 - Ground v=0  7  0 A2 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 23:<LineList>
 10.5 A1  1   9.5 A2  1   13554.3650   13554.3597      0.0053 1       .00028      0 : qR0(7)10.5,9.5 : Ground v=0  8  0 A1 10.5 - Ground v=0  7  0 A2 9.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 24:<LineList>
 11.5 A1  1  10.5 A2  1   16942.3180   16942.3095      0.0085 1       8.9e-5      0 : qR0(9)11.5,10.5 : Ground v=0 10  0 A1 11.5 - Ground v=0  9  0 A2 10.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 25:<LineList>
  3.5  E  9   2.5  E  7   10156.0710   10156.0845     -0.0135 1       .00016      0 : qR1(5)3.5,2.5 : Ground v=0  6  1 E 3.5 - Ground v=0  5  1 E 2.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 26:<LineList>
  4.5  E 10   3.5  E  9   11850.1710   11850.1758     -0.0048 1       .00014      0 : qR1(6)4.5,3.5 : Ground v=0  7  1 E 4.5 - Ground v=0  6  1 E 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 27:<LineList>
  5.5  E  8   4.5  E  8   11836.5160   11836.5211     -0.0051 1       .00017      0 : qR1(6)5.5,4.5 : Ground v=0  7  1 E 5.5 - Ground v=0  6  1 E 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 28:<LineList>
  5.5  E  4   4.5  E  3    8450.1030    8450.1074     -0.0044 1       .00029      0 : qR1(4)5.5,4.5 : Ground v=0  5  1 E 5.5 - Ground v=0  4  1 E 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 29:<LineList>
  5.5  E  6   4.5  E  6   10137.3780   10137.3814     -0.0034 1       .00023      0 : qR1(5)5.5,4.5 : Ground v=0  6  1 E 5.5 - Ground v=0  5  1 E 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 30:<LineList>
  5.5  E 10   4.5  E 10   13544.4450   13544.4241      0.0209 1       .00011      0 : qR1(7)5.5,4.5 : Ground v=0  8  1 E 5.5 - Ground v=0  7  1 E 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 31:<LineList>
  6.5  E  8   5.5  E  8   13534.5060   13534.5083     -0.0023 1       .00013      0 : qR1(7)6.5,5.5 : Ground v=0  8  1 E 6.5 - Ground v=0  7  1 E 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 32:<LineList>
  6.5  E  6   5.5  E  6   11838.5370   11838.5294      0.0076 1        .0002      0 : qR1(6)6.5,5.5 : Ground v=0  7  1 E 6.5 - Ground v=0  6  1 E 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 33:<LineList>
  6.5  E  2   5.5  E  2    8476.0110    8476.0084      0.0026 1       .00037      0 : qR1(4)6.5,5.5 : Ground v=0  5  1 E 6.5 - Ground v=0  4  1 E 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 34:<LineList>
  7.5  E  1   6.5  E  1    8490.4510    8490.4566     -0.0056 1       .00045      0 : qR1(4)7.5,6.5 : Ground v=0  5  1 E 7.5 - Ground v=0  4  1 E 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 35:<LineList>
  7.5  E  6   6.5  E  6   13536.7130   13536.7220     -0.0090 1       .00015      0 : qR1(7)7.5,6.5 : Ground v=0  8  1 E 7.5 - Ground v=0  7  1 E 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 36:<LineList>
  7.5  E  2   6.5  E  2   10170.6980   10170.6988     -0.0008 1       .00034      0 : qR1(5)7.5,6.5 : Ground v=0  6  1 E 7.5 - Ground v=0  5  1 E 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 37:<LineList>
  8.5  E  1   7.5  E  1   10176.8180   10176.8092      0.0088 1        .0004      0 : qR1(5)8.5,7.5 : Ground v=0  6  1 E 8.5 - Ground v=0  5  1 E 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 38:<LineList>
  8.5  E  2   7.5  E  2   11863.5760   11863.5765     -0.0005 1       .00027      0 : qR1(6)8.5,7.5 : Ground v=0  7  1 E 8.5 - Ground v=0  6  1 E 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 39:<LineList>
  8.5  E  4   7.5  E  4   13546.1930   13546.1950     -0.0020 1       .00017      0 : qR1(7)8.5,7.5 : Ground v=0  8  1 E 8.5 - Ground v=0  7  1 E 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 40:<LineList>
  9.5  E  1   8.5  E  1   11866.1200   11866.1231     -0.0031 1       .00031      0 : qR1(6)9.5,8.5 : Ground v=0  7  1 E 9.5 - Ground v=0  6  1 E 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 41:<LineList>
  9.5  E  7   8.5  E  7   16928.7760   16928.7889     -0.0129 1       5.7e-5      0 : qR1(9)9.5,8.5 : Ground v=0 10  1 E 9.5 - Ground v=0  9  1 E 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 42:<LineList>
 10.5  E  1   9.5  E  1   13556.9700   13556.9666      0.0034 1       .00022      0 : qR1(7)10.5,9.5 : Ground v=0  8  1 E 10.5 - Ground v=0  7  1 E 9.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 43:<LineList>
 11.5  E  3  10.5  E  3   16941.2180   16941.2172      0.0008 1         7e-5      0 : qR1(9)11.5,10.5 : Ground v=0 10  1 E 11.5 - Ground v=0  9  1 E 10.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 44:<LineList>
 12.5  E  1  11.5  E  1   16940.8890   16940.8741      0.0149 1       7.6e-5      0 : qR1(9)12.5,11.5 : Ground v=0 10  1 E 12.5 - Ground v=0  9  1 E 11.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 45:<LineList>
  4.5  E 12   3.5  E 11   11869.6690   11869.6756     -0.0066 1       6.8e-5      0 : qR2(6)4.5,3.5 : Ground v=0  7  2 E 4.5 - Ground v=0  6  2 E 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 46:<LineList>
  4.5  E 11   3.5  E 10   10151.2300   10151.2305     -0.0005 1       8.8e-5      0 : qR2(5)4.5,3.5 : Ground v=0  6  2 E 4.5 - Ground v=0  5  2 E 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 47:<LineList>
  4.5  E  9   3.5  E  8    8430.0260    8430.0069      0.0191 1        .0001      0 : qR2(4)4.5,3.5 : Ground v=0  5  2 E 4.5 - Ground v=0  4  2 E 3.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 48:<LineList>
  5.5  E  7   4.5  E  7    8419.4700    8419.4831     -0.0131 1       .00013      0 : qR2(4)5.5,4.5 : Ground v=0  5  2 E 5.5 - Ground v=0  4  2 E 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 49:<LineList>
  6.5  E  9   5.5  E  9   11833.9570   11833.9543      0.0027 1       9.4e-5      0 : qR2(6)6.5,5.5 : Ground v=0  7  2 E 6.5 - Ground v=0  6  2 E 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 50:<LineList>
  6.5  E 10   5.5  E 11   13538.3800   13538.3762      0.0038 1       6.2e-5      0 : qR2(7)6.5,5.5 : Ground v=0  8  2 E 6.5 - Ground v=0  7  2 E 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 51:<LineList>
  6.5  E  7   5.5  E  7   10133.2670   10133.2669      0.0001 1       .00013      0 : qR2(5)6.5,5.5 : Ground v=0  6  2 E 6.5 - Ground v=0  5  2 E 5.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 52:<LineList>
  7.5  E  5   6.5  E  5   10150.4390   10150.4327      0.0063 1       .00016      0 : qR2(5)7.5,6.5 : Ground v=0  6  2 E 7.5 - Ground v=0  5  2 E 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 53:<LineList>
  7.5  E  8   6.5  E  9   13532.8470   13532.8430      0.0040 1       7.1e-5      0 : qR2(7)7.5,6.5 : Ground v=0  8  2 E 7.5 - Ground v=0  7  2 E 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 54:<LineList>
  7.5  E  7   6.5  E  7   11837.7570   11837.7565      0.0005 1       .00011      0 : qR2(6)7.5,6.5 : Ground v=0  7  2 E 7.5 - Ground v=0  6  2 E 6.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 55:<LineList>
  8.5  E  5   7.5  E  5   11851.9740   11851.9707      0.0033 1       .00013      0 : qR2(6)8.5,7.5 : Ground v=0  7  2 E 8.5 - Ground v=0  6  2 E 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 56:<LineList>
  8.5  E  3   7.5  E  3   10194.0870   10194.0921     -0.0051 1       .00018      0 : qR2(5)8.5,7.5 : Ground v=0  6  2 E 8.5 - Ground v=0  5  2 E 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 57:<LineList>
  9.5  E  3   8.5  E  3   11877.4290   11877.4267      0.0023 1       .00015      0 : qR2(6)9.5,8.5 : Ground v=0  7  2 E 9.5 - Ground v=0  6  2 E 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 58:<LineList>
 10.5  E  2   9.5  E  3   13564.7410   13564.7331      0.0079 1        .0001      0 : qR2(7)10.5,9.5 : Ground v=0  8  2 E 10.5 - Ground v=0  7  2 E 9.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 59:<LineList>
  5.5 A1  9   4.5 A2  8   13577.8280   13577.8369     -0.0089 1       1.6e-5      0 : qR3(7)5.5,4.5 : Ground v=0  8  3 A1 5.5 - Ground v=0  7  3 A2 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 60:<LineList>
  5.5 A2  9   4.5 A1  8   13577.8280   13577.8369     -0.0089 1       1.6e-5      0 : qR3(7)5.5,4.5 : Ground v=0  8  3 A2 5.5 - Ground v=0  7  3 A1 4.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 61:<LineList>
  8.5 A1  3   7.5 A2  3   10222.0010   10222.0051     -0.0041 1         5e-5      0 : qR3(5)8.5,7.5 : Ground v=0  6  3 A1 8.5 - Ground v=0  5  3 A2 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 62:<LineList>
  8.5 A2  3   7.5 A1  3   10222.0010   10222.0051     -0.0041 1         5e-5      0 : qR3(5)8.5,7.5 : Ground v=0  6  3 A2 8.5 - Ground v=0  5  3 A1 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 63:<LineList>
  8.5 A1  4   7.5 A2  5   11833.5940   11833.5895      0.0045 1       3.7e-5      0 : qR3(6)8.5,7.5 : Ground v=0  7  3 A1 8.5 - Ground v=0  6  3 A2 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 64:<LineList>
  8.5 A2  4   7.5 A1  4   11833.5940   11833.5895      0.0045 1       3.7e-5      0 : qR3(6)8.5,7.5 : Ground v=0  7  3 A2 8.5 - Ground v=0  6  3 A1 7.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 65:<LineList>
  9.5 A1  2   8.5 A2  3   11895.8980   11895.8881      0.0099 1       4.2e-5      0 : qR3(6)9.5,8.5 : Ground v=0  7  3 A1 9.5 - Ground v=0  6  3 A2 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 66:<LineList>
  9.5 A1  4   8.5 A2  4   13537.3940   13537.3738      0.0202 1       2.7e-5      0 : qR3(7)9.5,8.5 : Ground v=0  8  3 A1 9.5 - Ground v=0  7  3 A2 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 67:<LineList>
  9.5 A2  4   8.5 A1  4   13537.3940   13537.3738      0.0202 1       2.7e-5      0 : qR3(7)9.5,8.5 : Ground v=0  8  3 A2 9.5 - Ground v=0  7  3 A1 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 68:<LineList>
  9.5 A2  3   8.5 A1  3   11895.8980   11895.8881      0.0099 1       4.2e-5      0 : qR3(6)9.5,8.5 : Ground v=0  7  3 A2 9.5 - Ground v=0  6  3 A1 8.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 69:<LineList>
 10.5 A1  3   9.5 A2  3   13577.5040   13577.4998      0.0042 1       3.1e-5      0 : qR3(7)10.5,9.5 : Ground v=0  8  3 A1 10.5 - Ground v=0  7  3 A2 9.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 70:<LineList>
 10.5 A2  2   9.5 A1  2   13577.5040   13577.4998      0.0042 1       3.1e-5      0 : qR3(7)10.5,9.5 : Ground v=0  8  3 A2 10.5 - Ground v=0  7  3 A1 9.5 : 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311 - 8X_3dropsH2O_1divCF3I_balance1barAr_86134_310311.ovr   : 71:<LineList>
  6.5  E  5   5.5  E  5    8437.1009    8437.0948      0.0061 1       .00029      0 : qR2(4)6.5,5.5 : v=0  5  2 E 6.5 - v=0  4  2 E 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 72:<LineList>
  5.5 A2  2   4.5 A1  2    8459.9603    8459.9632     -0.0029 1       .00068      0 : qR0(4)5.5,4.5 : v=0  5  0 A2 5.5 - v=0  4  0 A1 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 73:<LineList>
  3.5 A1  3   2.5 A2  3   10145.1625   10145.1746     -0.0121 1       .00036      0 : qR0(5)3.5,2.5 : v=0  6  0 A1 3.5 - v=0  5  0 A2 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 74:<LineList>
  6.5  E  4   5.5  E  4   10152.5231   10152.5281     -0.0050 1        .0005      0 : qR1(5)6.5,5.5 : v=0  6  1 E 6.5 - v=0  5  1 E 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 75:<LineList>
  5.5  E  9   4.5  E  9   10132.8264   10132.8330     -0.0066 1       .00019      0 : qR2(5)5.5,4.5 : v=0  6  2 E 5.5 - v=0  5  2 E 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 76:<LineList>
  6.5 A2  7   5.5 A1  7   11826.1142   11826.1180     -0.0038 1       4.7e-5      0 : qR3(6)6.5,5.5 : v=0  7  3 A2 6.5 - v=0  6  3 A1 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 77:<LineList>
  6.5 A1  7   5.5 A2  7   11826.1142   11826.1180     -0.0038 1       4.7e-5      0 : qR3(6)6.5,5.5 : v=0  7  3 A1 6.5 - v=0  6  3 A2 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 78:<LineList>
  4.5  E  3   3.5  E  3    6736.7779    6736.7756      0.0023 1       .00044      0 : qR1(3)4.5,3.5 : v=0  4  1 E 4.5 - v=0  3  1 E 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 79:<LineList>
  4.5 A1  2   3.5 A2  2    6751.2197    6751.2158      0.0039 1       .00058      0 : qR0(3)4.5,3.5 : v=0  4  0 A1 4.5 - v=0  3  0 A2 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 80:<LineList>
  5.5  E  2   4.5  E  2    6773.7170    6773.7218     -0.0048 1       .00059      0 : qR1(3)5.5,4.5 : v=0  4  1 E 5.5 - v=0  3  1 E 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 81:<LineList>
  5.5 A1  1   4.5 A2  1    6805.8890    6805.8961     -0.0071 1       .00079      0 : qR0(3)5.5,4.5 : v=0  4  0 A1 5.5 - v=0  3  0 A2 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 82:<LineList>
  6.5  E  1   5.5  E  1    6810.5345    6810.5370     -0.0025 1       .00076      0 : qR1(3)6.5,5.5 : v=0  4  1 E 6.5 - v=0  3  1 E 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 83:<LineList>
  8.5 A2  5   7.5 A1  5   13523.0199   13523.0180      0.0019 1       4.2e-5      0 : qR3(7)8.5,7.5 : v=0  8  3 A2 8.5 - v=0  7  3 A1 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 84:<LineList>
  8.5 A1  6   7.5 A2  6   13523.0199   13523.0180      0.0019 1       4.2e-5      0 : qR3(7)8.5,7.5 : v=0  8  3 A1 8.5 - v=0  7  3 A2 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 85:<LineList>
  7.5 A2  7   6.5 A1  7   13526.2632   13526.2637     -0.0005 1       3.7e-5      0 : qR3(7)7.5,6.5 : v=0  8  3 A2 7.5 - v=0  7  3 A1 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 86:<LineList>
  7.5 A1  7   6.5 A2  7   13526.2632   13526.2637     -0.0005 1       3.7e-5      0 : qR3(7)7.5,6.5 : v=0  8  3 A1 7.5 - v=0  7  3 A2 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 87:<LineList>
  9.5  E  4   8.5  E  5   13548.9137   13548.9155     -0.0018 1       .00016      0 : qR2(7)9.5,8.5 : v=0  8  2 E 9.5 - v=0  7  2 E 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 88:<LineList>
  9.5  E  2   8.5  E  2   13556.0670   13556.0826     -0.0156 1       .00034      0 : qR1(7)9.5,8.5 : v=0  8  1 E 9.5 - v=0  7  1 E 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 89:<LineList>
  7.5 A2  4   6.5 A1  4   15230.3539   15230.3709     -0.0170 1       .00019      0 : qR0(8)7.5,6.5 : v=0  9  0 A2 7.5 - v=0  8  0 A1 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 90:<LineList>
  8.5  E  7   7.5  E  6   15233.2454   15233.2546     -0.0092 1       .00017      0 : qR1(8)8.5,7.5 : v=0  9  1 E 8.5 - v=0  8  1 E 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 91:<LineList>
  7.5  E 10   6.5  E 10   15233.2454   15233.2626     -0.0172 1       7.3e-5      0 : qR2(8)7.5,6.5 : v=0  9  2 E 7.5 - v=0  8  2 E 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 92:<LineList>
  8.5 A2  2   7.5 A1  2   15234.3012   15234.3025     -0.0013 1       .00022      0 : qR0(8)8.5,7.5 : v=0  9  0 A2 8.5 - v=0  8  0 A1 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 93:<LineList>
  7.5 A2  8   6.5 A1  8   15236.8887   15236.9085     -0.0198 1       2.2e-5      0 : qR3(8)7.5,6.5 : v=0  9  3 A2 7.5 - v=0  8  3 A1 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 94:<LineList>
  7.5 A1  8   6.5 A2  8   15236.8887   15236.9085     -0.0198 1       2.2e-5      0 : qR3(8)7.5,6.5 : v=0  9  3 A1 7.5 - v=0  8  3 A2 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr   : 95:<LineList>
```

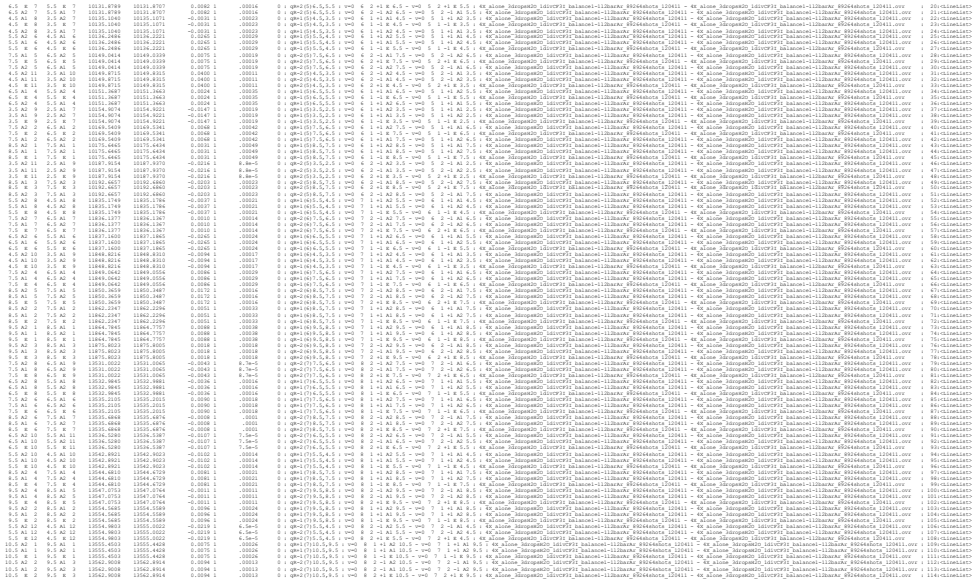


```
102 Observations,  4 Parameters
Initial Average Error: 0.00843866317244115
Predicted New Error:   0.00843866317243777
Parameters:
  # Old                  New                  Std Dev    Change/Std Sens    Summary              Name
  1 846.820303741271     846.820303739713     .00018511    0.0000  1.45e-5 846.82030(19)        v=0 B
  2 .000143068644503587 .000143068633082497 1.3268e-6    0.0000  1.1e-7  1.431(13)e-4         v=0 DJ
  3 .00192085550456349  .00192085546204788  1.6067e-5    0.0000  3.04e-6 1.921(16)e-3         v=0 DJK
  4 -2199.27458373478   -2199.27458361905   .08422883    0.0000  .020797 -2199.275(84)        Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.910   1.000
  3   0.327   0.059   1.000
  4  -0.181  -0.126  -0.145   1.000
```

$H_2{}^{16}O\cdots ICF_3$, Symmetric top, m=±1 transitions.

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_H2O_sym_m=1_only.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei        1
      JAdjustSym     False
      BlockMatrix    True
      PointGroup     C3v
      AlternateBasis False
      wt(A1,A2)      1
      wt(E)          1
      (Wt2)          1
      (Wt3)          1
      (Wt4)          1
      (Wt5)          1
      (Wt6)          1
      (Wt7)          1
      (Wt8)          1
      (Wt9)          1
      (Wt10)         1
      (Wt11)         1
      (Wt12)         1
      (Wt13)         1
      Abundance 1
      SymmetricManifold: Ground
        Initial        True
        Colour         Green
        EigenSearch    True
        LimitSearch    False
        AutoQConverge  True
        UsePopParams   False
        SymmetricTop: v=0
          Symmetry E
          Kmin     1
          Kmax     2
          B    846.727662182102           Float
          C    5600
          DJ  0.000111189519472145        Float
          DJK 0.00851677485027583         Float
          symmetricTopNucleus: Nucleus1
            Spin   2.5
            AsNext False
            eQq -2198.92016694114           Float
        <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
        <J,N,K,l|C|J,N,K,l> = K^2
        <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
        <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
      TransitionMoments: <Ground|mu|Ground>
        CartesianTransitionMoment: <v=0|a|v=0>
          Axis a
          Strength 1
```





```
114 Observations,  4 Parameters
Initial Average Error: 0.0144359207881988
Predicted New Error:   0.0144359207881965
Parameters:
  # Old                  New                  Std Dev   Change/Std Sens    Summary              Name
  1 846.727662182102     846.727662181133     .00041254    0.0000  2.66e-5 846.72766(41)        v=0 B
  2 .000111189519472145 .000111189503220865 3.7793e-6    0.0000  2.54e-7 1.112(38)e-4         v=0 DJ
  3 .00851677485027583   .00851677515360325   6.809e-5     0.0000  9.83e-6 8.517(68)e-3         v=0 DJK
  4 -2198.92016694114    -2198.92016687859    .16838698    0.0000  .042567 -2198.92(17)         Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.893   1.000
  3   0.263  -0.123   1.000
  4  -0.268  -0.190  -0.079   1.000
```

$H_2{}^{18}O\cdots ICF_3$, Symmetric top, m=0 transitions.

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_18H2O_sym_m=0_only.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei         1
      JAdjustSym      False
      BlockMatrix     True
      PointGroup      C3v
      AlternateBasis False
      wt(A1,A2)       1
      wt(E)           1
      (Wt2)           1
      (Wt3)           1
      (Wt4)           1
      (Wt5)           1
      (Wt6)           1
      (Wt7)           1
      (Wt8)           1
      (Wt9)           1
      (Wt10)          1
      (Wt11)          1
      (Wt12)          1
      (Wt13)          1
      Abundance 1
      SymmetricManifold: Ground
        Initial        True
        Colour         Green
        EigenSearch    True
        LimitSearch    False
        AutoQConverge True
        UsePopParams   False
```

```
          SymmetricTop: v=0
            Symmetry A1
            Kmin      all
            Kmax      all
            B    812.061023726328           Float
            C    5600
            DJ   0.000136047571600479       Float
            DJK 0.00183993544197199         Float
            symmetricTopNucleus: Nucleus1
              Spin    2.5
              AsNext False
              eQq -2198.81503479962           Float
          <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
          <J,N,K,l|C|J,N,K,l> = K^2
          <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
          <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
        TransitionMoments: <Ground|mu|Ground>
          CartesianTransitionMoment: <v=0|a|v=0>
            Axis a
            Strength 1
```

```
Residuals before fit for SymmetricTop for the Ground manifold
   J' S' #'    J" S" #"    Observed    Calculated    Obs-Calc  StdDev
  8.5  E  8   7.5  E  8  14604.4790  14604.4484    0.0306 1   8.7e-5   0 : qR2(8)8.5,7.5 : v=0  9  2 E 8.5 - v=0  8  2 E 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   1:<LineList>
  7.5 A2  4   6.5 A1  3  14604.7010  14604.7130   -0.0120 1    .0002   0 : qR0(8)7.5,6.5 : v=0  9  0 A2 7.5 - v=0  8  0 A1 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   2:<LineList>
  7.5  E  9   6.5  E  8  14605.4080  14605.4351   -0.0271 1   .00016   0 : qR1(8)7.5,6.5 : v=0  9  1 E 7.5 - v=0  8  1 E 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   3:<LineList>
  8.5 A2  2   7.5 A1  2  14608.6200  14608.6348   -0.0148 1   .00023   0 : qR0(8)8.5,7.5 : v=0  9  0 A2 8.5 - v=0  8  0 A1 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   4:<LineList>
  9.5  E  6   8.5  E  6  14609.1470  14609.1236    0.0234 1   9.8e-5   0 : qR2(8)9.5,8.5 : v=0  9  2 E 9.5 - v=0  8  2 E 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   5:<LineList>
  6.5 A2  5   5.5 A1  4  14610.1330  14610.1550   -0.0220 1   .00018   0 : qR0(8)6.5,5.5 : v=0  9  0 A2 6.5 - v=0  8  0 A1 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   6:<LineList>
 10.5 A2  4   9.5 A1  4  14610.5890  14610.5656    0.0234 1   3.2e-5   0 : qR3(8)10.5,9.5 : v=0  9  3 A2 10.5 - v=0  8  3 A1 9.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   7:<LineList>
 10.5 A1  4   9.5 A2  4  14610.5890  14610.5656    0.0234 1   3.2e-5   0 : qR3(8)10.5,9.5 : v=0  9  3 A1 10.5 - v=0  8  3 A2 9.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   8:<LineList>
  7.5 A2  8   6.5 A1  8  14611.2610  14611.2637   -0.0027 1   2.3e-5   0 : qR3(8)7.5,6.5 : v=0  9  3 A2 7.5 - v=0  8  3 A1 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :   9:<LineList>
  7.5 A1  8   6.5 A2  8  14611.2610  14611.2637   -0.0027 1   2.3e-5   0 : qR3(8)7.5,6.5 : v=0  9  3 A1 7.5 - v=0  8  3 A2 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  10:<LineList>
  6.5  E 11   5.5  E 10  14612.9410  14612.9310    0.0100 1   .00014   0 : qR1(8)6.5,5.5 : v=0  9  1 E 6.5 - v=0  8  1 E 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  11:<LineList>
  9.5  E  5   8.5  E  4  14615.3010  14615.2957    0.0053 1    .0002   0 : qR1(8)9.5,8.5 : v=0  9  1 E 9.5 - v=0  8  1 E 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  12:<LineList>
 10.5 A2  1   9.5 A1  1  14624.5330  14624.5556   -0.0226 1   .00029   0 : qR0(8)10.5,9.5 : v=0  9  0 A2 10.5 - v=0  8  0 A1 9.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  13:<LineList>
 11.5  E  1  10.5  E  1  14623.0520  14623.0390    0.0130 1   .00025   0 : qR1(8)11.5,10.5 : v=0  9  1 E 11.5 - v=0  8  1 E 10.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  14:<LineList>
 11.5 A2  1  10.5 A1  1  14621.1850  14621.1763    0.0087 1   .00032   0 : qR0(8)11.5,10.5 : v=0  9  0 A2 11.5 - v=0  8  0 A1 10.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr :  15:<LineList>
 11.5  E  2  10.5  E  3  14628.6250  14628.5983    0.0267 1   .00012   0 : qR2(8)11.5,10.5 : v=0  9  2 E 11.5 - v=0  8  2 E 10.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  16:<LineList>
 11.5 A2  3  10.5 A1  3  14637.7810  14637.7688    0.0122 1   3.6e-5   0 : qR3(8)11.5,10.5 : v=0  9  3 A2 11.5 - v=0  8  3 A1 10.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr :  17:<LineList>
 11.5 A1  2  10.5 A2  2  14637.7810  14637.7688    0.0122 1   3.6e-5   0 : qR3(8)11.5,10.5 : v=0  9  3 A1 11.5 - v=0  8  3 A2 10.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr :  18:<LineList>
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 12.5 A1  3  11.5 A2  3  16256.5610  16256.5865   -0.0255 1   2.1e-5   0 : qR3(9)12.5,11.5 : v=0 10  3 A1 12.5 - v=0  9  3 A2 11.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr :  36:<LineList>
  5.5  E  7   4.5  E  7   8072.0030   8071.9999    0.0031 1   .00022   0 : qR2(4)5.5,4.5 : v=0  5  2 E 5.5 - v=0  4  2 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  37:<LineList>
  3.5 A2  3   2.5 A1  3   8073.4920   8073.4907    0.0013 1   .00039   0 : qR0(4)3.5,2.5 : v=0  5  0 A2 3.5 - v=0  4  0 A1 2.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  38:<LineList>
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  5.5  E  4   4.5  E  3   8102.4730   8102.4656    0.0074 1    .0005   0 : qR1(4)5.5,4.5 : v=0  5  1 E 5.5 - v=0  4  1 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  44:<LineList>
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  2.5  E  7   1.5  E  4   8115.6440   8115.6568   -0.0128 1   .00023   0 : qR1(4)2.5,1.5 : v=0  5  1 E 2.5 - v=0  4  1 E 1.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  46:<LineList>
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  6.5 A2  1   5.5 A1  1   8142.3840   8142.3800    0.0040 1   .00082   0 : qR0(4)6.5,5.5 : v=0  5  0 A2 6.5 - v=0  4  0 A1 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  48:<LineList>
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  5.5 A2  7   4.5 A1  6   9707.9010   9707.9037   -0.0027 1   4.9e-5   0 : qR3(5)5.5,4.5 : v=0  6  3 A2 5.5 - v=0  5  3 A1 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  53:<LineList>
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  4.5 A1  3   3.5 A2  3   9714.2760   9714.2775   -0.0015 1   .00043   0 : qR0(5)4.5,3.5 : v=0  6  0 A1 4.5 - v=0  5  0 A2 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  55:<LineList>
  5.5  E  9   4.5  E  9   9715.7010   9715.7379   -0.0369 1   .00018   0 : qR2(5)5.5,4.5 : v=0  6  2 E 5.5 - v=0  5  2 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  56:<LineList>
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  4.5  E  8   3.5  E  7   9719.1450   9719.1381    0.0069 1   .00033   0 : qR1(5)4.5,3.5 : v=0  6  1 E 4.5 - v=0  5  1 E 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  58:<LineList>
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  8.5  E  3   7.5  E  3   9777.0850   9777.0826    0.0024 1   .00032   0 : qR2(5)8.5,7.5 : v=0  6  2 E 8.5 - v=0  5  2 E 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  70:<LineList>
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  6.5 A2  7   5.5 A1  7  11339.5460  11339.5519   -0.0059 1   4.7e-5   0 : qR3(6)6.5,5.5 : v=0  7  3 A2 6.5 - v=0  6  3 A1 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  73:<LineList>
  6.5 A1  7   5.5 A2  7  11339.5460  11339.5519   -0.0059 1   4.7e-5   0 : qR3(6)6.5,5.5 : v=0  7  3 A1 6.5 - v=0  6  3 A2 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  74:<LineList>
  8.5 A2  4   7.5 A1  4  11346.8480  11346.8665   -0.0185 1   6.4e-5   0 : qR3(6)8.5,7.5 : v=0  7  3 A2 8.5 - v=0  6  3 A1 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  75:<LineList>
  8.5 A1  4   7.5 A2  5  11346.8480  11346.8665   -0.0185 1   6.4e-5   0 : qR3(6)8.5,7.5 : v=0  7  3 A1 8.5 - v=0  6  3 A2 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  76:<LineList>
  5.5 A2  3   4.5 A1  3  11347.4870  11347.4905   -0.0035 1   .00038   0 : qR0(6)5.5,4.5 : v=0  7  0 A2 5.5 - v=0  6  0 A1 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  77:<LineList>
  6.5  E  9   5.5  E  9  11347.3450  11347.3409    0.0041 1   .00017   0 : qR2(6)6.5,5.5 : v=0  7  2 E 6.5 - v=0  6  2 E 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  78:<LineList>
  5.5  E  8   4.5  E  8  11349.8770  11349.8846   -0.0076 1    .0003   0 : qR1(6)5.5,4.5 : v=0  7  1 E 5.5 - v=0  6  1 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  79:<LineList>
  7.5  E  7   6.5  E  7  11351.1460  11351.1419    0.0041 1   .00019   0 : qR2(6)7.5,6.5 : v=0  7  2 E 7.5 - v=0  6  2 E 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  80:<LineList>
  6.5 A2  2   5.5 A1  2  11353.3760  11353.3765   -0.0005 1   .00045   0 : qR0(6)6.5,5.5 : v=0  7  0 A2 6.5 - v=0  6  0 A1 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  81:<LineList>
  6.5  E  6   5.5  E  6  11351.8710  11351.8834   -0.0124 1   .00035   0 : qR1(6)6.5,5.5 : v=0  7  1 E 6.5 - v=0  6  1 E 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  82:<LineList>
  4.5 A2  3   3.5 A1  3  11357.1150  11357.1248   -0.0098 1   .00032   0 : qR0(6)4.5,3.5 : v=0  7  0 A2 4.5 - v=0  6  0 A1 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  83:<LineList>
  5.5  E 11   4.5  E 11  11357.1150  11357.1597   -0.0447 1   .00014   0 : qR2(6)5.5,4.5 : v=0  7  2 E 5.5 - v=0  6  2 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  84:<LineList>
  8.5  E  5   7.5  E  5  11365.3040  11365.2946    0.0094 1   .00023   0 : qR2(6)8.5,7.5 : v=0  7  2 E 8.5 - v=0  6  2 E 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  85:<LineList>
  4.5  E 10   3.5  E  9  11363.5270  11363.5410   -0.0140 1   .00025   0 : qR1(6)4.5,3.5 : v=0  7  1 E 4.5 - v=0  6  1 E 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  86:<LineList>
  7.5 A2  2   6.5 A1  2  11367.9400  11367.9376    0.0024 1   .00053   0 : qR0(6)7.5,6.5 : v=0  7  0 A2 7.5 - v=0  6  0 A1 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  87:<LineList>
  9.5 A2  1   8.5 A1  1  11375.7340  11375.7192    0.0148 1    .0007   0 : qR0(6)9.5,8.5 : v=0  7  0 A2 9.5 - v=0  6  0 A1 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  88:<LineList>
  8.5  E  2   7.5  E  2  11376.9530  11376.9561   -0.0031 1   .00048   0 : qR1(6)8.5,7.5 : v=0  7  1 E 8.5 - v=0  6  1 E 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  89:<LineList>
  9.5  E  1   8.5  E  1  11379.5440  11379.5375    0.0065 1   .00055   0 : qR1(6)9.5,8.5 : v=0  7  1 E 9.5 - v=0  6  1 E 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  90:<LineList>
  8.5 A2  1   7.5 A1  1  11380.9500  11380.9487    0.0013 1   .00062   0 : qR0(6)8.5,7.5 : v=0  7  0 A2 8.5 - v=0  6  0 A1 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  91:<LineList>
  4.5  E 12   3.5  E 11  11382.9860  11382.9985   -0.0125 1   .00012   0 : qR2(6)4.5,3.5 : v=0  7  2 E 4.5 - v=0  6  2 E 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  92:<LineList>
  9.5  E  3   8.5  E  3  11390.8710  11390.8701    0.0009 1   .00026   0 : qR2(6)9.5,8.5 : v=0  7  2 E 9.5 - v=0  6  2 E 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  93:<LineList>
  6.5 A1  3   5.5 A2  3  12977.1010  12977.0815    0.0195 1    .0003   0 : qR0(7)6.5,5.5 : v=0  8  0 A1 6.5 - v=0  7  0 A2 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  94:<LineList>
  7.5  E  8   6.5  E  9  12976.7130  12976.7126    0.0004 1   .00013   0 : qR2(7)7.5,6.5 : v=0  8  2 E 7.5 - v=0  7  2 E 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  95:<LineList>
  6.5  E  8   5.5  E  8  12978.3490  12978.3616   -0.0126 1   .00023   0 : qR1(7)6.5,5.5 : v=0  8  1 E 6.5 - v=0  7  1 E 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  96:<LineList>
  7.5  E  6   6.5  E  6  12980.5570  12980.5683   -0.0113 1   .00027   0 : qR1(7)7.5,6.5 : v=0  8  1 E 7.5 - v=0  7  1 E 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  97:<LineList>
  7.5 A1  2   6.5 A2  2  12981.8320  12981.8420   -0.0100 1   .00034   0 : qR0(7)7.5,6.5 : v=0  8  0 A1 7.5 - v=0  7  0 A2 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  98:<LineList>
  8.5  E  6   7.5  E  7  12981.3880  12981.3909   -0.0029 1   .00015   0 : qR2(7)8.5,7.5 : v=0  8  2 E 8.5 - v=0  7  2 E 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  99:<LineList>
  9.5 A2  4   8.5 A1  4  12981.1910  12981.1804    0.0106 1   4.8e-5   0 : qR3(7)9.5,8.5 : v=0  8  3 A2 9.5 - v=0  7  3 A1 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 100:<LineList>
  9.5 A1  4   8.5 A2  4  12981.1910  12981.1804    0.0106 1   4.8e-5   0 : qR3(7)9.5,8.5 : v=0  8  3 A1 9.5 - v=0  7  3 A2 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 101:<LineList>
  5.5 A1  4   4.5 A2  3  12984.1810  12984.1791    0.0019 1   .00026   0 : qR0(7)5.5,4.5 : v=0  8  0 A1 5.5 - v=0  7  0 A2 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 102:<LineList>
  5.5  E 10   4.5  E 10  12988.2730  12988.2802   -0.0072 1    .0002   0 : qR1(7)5.5,4.5 : v=0  8  1 E 5.5 - v=0  7  1 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 103:<LineList>
  8.5  E  4   7.5  E  4  12990.0180  12990.0445   -0.0265 1   .00031   0 : qR1(7)8.5,7.5 : v=0  8  1 E 8.5 - v=0  7  1 E 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 104:<LineList>
  8.5 A1  2   7.5 A2  2  12992.9280  12992.9227    0.0053 1   .00039   0 : qR0(7)8.5,7.5 : v=0  8  0 A1 8.5 - v=0  7  0 A2 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 105:<LineList>
 10.5 A1  1   9.5 A2  1  12998.2540  12998.2429    0.0111 1    .0005   0 : qR0(7)10.5,9.5 : v=0  8  0 A1 10.5 - v=0  7  0 A2 9.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 106:<LineList>
 10.5  E  1   9.5  E  1  13000.8680  13000.8574    0.0106 1   .00039   0 : qR1(7)10.5,9.5 : v=0  8  1 E 10.5 - v=0  7  1 E 9.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 107:<LineList>
  5.5  E 12   4.5  E 12  13000.6820  13000.6741    0.0079 1   9.6e-5   0 : qR2(7)5.5,4.5 : v=0  8  2 E 5.5 - v=0  7  2 E 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 108:<LineList>
  9.5 A1  1   8.5 A2  1  13002.4230  13002.3978    0.0252 1   .00045   0 : qR0(7)9.5,8.5 : v=0  8  0 A1 9.5 - v=0  7  0 A2 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 109:<LineList>
 10.5  E  3   9.5  E  3  13008.6570  13008.6442    0.0128 1   .00019   0 : qR2(7)10.5,9.5 : v=0  8  2 E 10.5 - v=0  7  2 E 9.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 110:<LineList>
108 Observations,  4 Parameters
Initial Average Error:  0.0136727363243136
Predicted New Error:    0.0136727363243097
Parameters:
  # Old                  New                  Std Dev     Change/Std Sens     Summary              Name
  1 812.061023726328     812.061023727903     .00029539     0.0000   2.24e-5  812.06102(30)        v=0 B
  2 .000136047571600479  .000136047579363972  1.9831e-6     0.0000   1.55e-7  1.360(20)e-4         v=0 DJ
  3 .00183993544197199   .00183993558800294   2.4026e-5     0.0000   4.58e-6  1.840(24)e-3         v=0 DJK
  4 -2198.81503479962    -2198.8150350234     .15772531     0.0000   .036698  -2198.82(16)         Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.916   1.000
  3   0.154  -0.119   1.000
  4  -0.415  -0.381   0.057   1.000
```
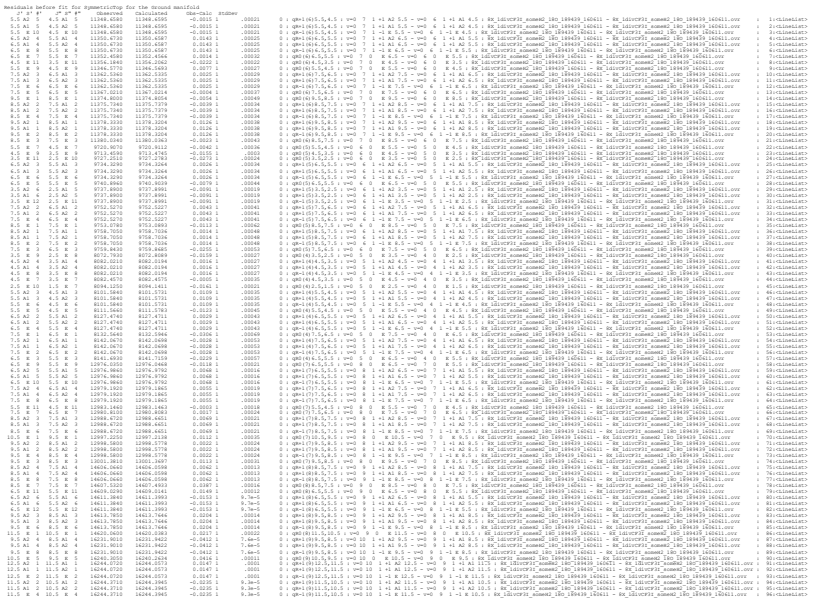

$H_2{}^{18}O\cdots ICF_3$, Symmetric top, $m=\pm1$ transitions.

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_18H2O_sym_m=1_only.pgo
  Units                 MHz
  PrintLevel            Detail
  Precision             4
  BasisOrder            boDefault
  QuantumNumberFormat J
  FitCycles             1
  FitDetails            False
  AutoReplot            True
  AllowComplex          False
  NoLineList            False
  ShowEstUnc            False
  ShowDerivatives       False
  SVDThresh      1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei          1
      JAdjustSym      False
      BlockMatrix     True
```

```
  PointGroup     C3v
  AlternateBasis False
  wt(A1,A2)      1
  wt(E)          1
  (Wt2)          1
  (Wt3)          1
  (Wt4)          1
  (Wt5)          1
  (Wt6)          1
  (Wt7)          1
  (Wt8)          1
  (Wt9)          1
  (Wt10)         1
  (Wt11)         1
  (Wt12)         1
  (Wt13)         1
  Abundance 1
  SymmetricManifold: Ground
    Initial        True
    Colour         Green
    EigenSearch    True
    LimitSearch    False
    AutoQConverge  True
    UsePopParams   False
    SymmetricTop: v=0
      Symmetry E
      Kmin     0
      Kmax     1
      B    811.992368396743          Float
      C    5600
      DJ  0.000102932498267071       Float
      DJK 0.02358837396537           Float
      symmetricTopNucleus: Nucleus1
        Spin   2.5
        AsNext False
        eQq -2199.3681298889           Float
    <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
    <J,N,K,l|C|J,N,K,l> = K^2
    <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
    <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
  TransitionMoments: <Ground|mu|Ground>
    CartesianTransitionMoment: <v=0|a|v=0>
      Axis a
      Strength 1
```



```
96 Observations,  4 Parameters
Initial Average Error: 0.0149686401674127
Predicted New Error:   0.0149686401674107
Parameters:
  # Old                  New                Std Dev   Change/Std Sens    Summary              Name
  1 811.992368396743     811.992368396256   .00033648    0.0000  2.55e-5 811.99237(34)        v=0 B
  2 .000102932498267071  .000102932501317286 2.2172e-6    0.0000  1.85e-7 1.029(22)e-4         v=0 DJ
  3 .02358837396537      .0235883727962081  .00024242     0.0000  2.95e-5 0.02359(24)          v=0 DJK
  4 -2199.3681298889     -2199.36812982192  .22764926     0.0000  .053014 -2199.37(23)         Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.779   1.000
  3   0.416  -0.150   1.000
  4  -0.256  -0.156  -0.078   1.000
```

HDO···ICF_3, symmetric top, *m*=0 transitions

```
Pgopher 7.1.187 04 Apr 2011 21:20
```

```
Mixture: CF3I_HDO_GROUND.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat  J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh     1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei         1
      JAdjustSym      False
      BlockMatrix     True
      PointGroup      C3v
      AlternateBasis  False
      wt(A1,A2)       1
      wt(E)           1
      (Wt2)           1
      (Wt3)           1
      (Wt4)           1
      (Wt5)           1
      (Wt6)           1
      (Wt7)           1
      (Wt8)           1
      (Wt9)           1
      (Wt10)          1
      (Wt11)          1
      (Wt12)          1
      (Wt13)          1
      Abundance 1
      SymmetricManifold: Ground
        Initial       True
        Colour        Green
        EigenSearch   True
        LimitSearch   False
        AutoQConverge True
        UsePopParams  False
        SymmetricTop: v=0
          Symmetry A1
          Kmin      all
          Kmax      all
          B    823.299004985202            Float
          C    5600
          DJ   0.000138464032638431        Float
          DJK  0.00207071486611839         Float
          symmetricTopNucleus: Nucleus1
            Spin    2.5
            AsNext False
            eQq -2199.20785496269            Float
        <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
        <J,N,K,l|C|J,N,K,l> = K^2
        <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
        <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
      TransitionMoments: <Ground|mu|Ground>
        CartesianTransitionMoment: <v=0|a|v=0>
          Axis a
          Strength 1
```

Residuals before fit for SymmetricTop for the Ground manifold

```
      J' S' #'    J" S" #"     Observed    Calculated      Obs-Calc  StdDev
  4.5 A1  2   3.5 A2  2     6562.8750     6562.8620     0.0130 1    .00056    0 : qR0(3)4.5,3.5 : v=0  4  0 A1 4.5 - v=0  3  0 A2 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   1:<LineList>
  4.5 A1  2   4.5 A2  1     6584.0000     6584.0174    -0.0174 1    .00015    0 : qR0(3)4.5,4.5 : v=0  4  0 A1 4.5 - v=0  3  0 A2 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   2:<LineList>
  5.5  E  2   4.5  E  2     6585.4300     6585.4222     0.0078 1    .00057    0 : qR1(3)5.5,4.5 : v=0  4  1 E 5.5 - v=0  3  1 E 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   3:<LineList>
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  5.5 A1  1   4.5 A2  1     6617.7710     6617.7642     0.0068 1    .00076    0 : qR0(3)5.5,4.5 : v=0  4  0 A1 5.5 - v=0  3  0 A2 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   5:<LineList>
  6.5  E  1   5.5  E  1     6622.4710     6622.4712    -0.0002 1    .00073    0 : qR1(3)6.5,5.5 : v=0  4  1 E 6.5 - v=0  3  1 E 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   6:<LineList>
  3.5 A2  3   2.5 A1  3     8185.8540     8185.8597    -0.0057 1     .0004    0 : qR0(4)3.5,2.5 : v=0  5  0 A2 3.5 - v=0  4  0 A1 2.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   7:<LineList>
  4.5 A2  6   3.5 A1  5     8194.4130     8194.4090     0.0040 1    4.2e-5    0 : qR3(4)4.5,3.5 : v=0  5  3 A2 4.5 - v=0  4  3 A1 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :   8:<LineList>
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  4.5  E  9   3.5  E  8     8194.7750     8194.7799    -0.0049 1    .00017    0 : qR2(4)4.5,3.5 : v=0  5  2 E 4.5 - v=0  4  2 E 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  10:<LineList>
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  7.5 A2  1   6.5 A1  1     8245.6340     8245.6252     0.0088 1    .00101    0 : qR0(4)7.5,6.5 : v=0  5  0 A2 7.5 - v=0  4  0 A1 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  18:<LineList>
  6.5 A2  1   5.5 A1  1     8254.7570     8254.7482     0.0088 1    .00083    0 : qR0(4)6.5,5.5 : v=0  5  0 A2 6.5 - v=0  4  0 A1 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  19:<LineList>
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  7.5 A1  3   6.5 A2  3     8328.1120     8328.1065     0.0055 1    8.2e-5    0 : qR3(4)7.5,6.5 : v=0  5  3 A1 7.5 - v=0  4  3 A2 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  21:<LineList>
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  6.5 A1  6   5.5 A2  6     9818.2150     9818.2076     0.0074 1    6.1e-5    0 : qR3(5)6.5,5.5 : v=0  6  3 A1 6.5 - v=0  5  3 A2 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  23:<LineList>
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  5.5 A2  7   4.5 A1  6     9842.7040     9842.7062    -0.0022 1      5e-5    0 : qR3(5)5.5,4.5 : v=0  6  3 A2 5.5 - v=0  5  3 A1 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  27:<LineList>
  5.5 A1  7   4.5 A2  6     9842.7040     9842.7062    -0.0022 1      5e-5    0 : qR3(5)5.5,4.5 : v=0  6  3 A1 5.5 - v=0  5  3 A2 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  28:<LineList>
  4.5 A1  3   3.5 A2  3     9849.1290     9849.1302    -0.0012 1    .00043    0 : qR0(5)4.5,3.5 : v=0  6  0 A1 4.5 - v=0  5  0 A2 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  29:<LineList>
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  3.5 A1  3   2.5 A2  3     9862.9160     9862.9268    -0.0108 1    .00035    0 : qR0(5)3.5,2.5 : v=0  6  0 A1 3.5 - v=0  5  0 A2 2.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  35:<LineList>
  7.5  E  5   6.5  E  5     9868.1050     9868.0936     0.0114 1    .00027    0 : qR2(5)7.5,6.5 : v=0  6  2 E 7.5 - v=0  5  2 E 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  36:<LineList>
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  6.5  E  4   5.5  E  4     9870.2520     9870.2479     0.0041 1    .00049    0 : qR1(5)6.5,5.5 : v=0  6  1 E 6.5 - v=0  5  1 E 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  38:<LineList>
  3.5  E  9   2.5  E  7     9873.8070     9873.8149    -0.0079 1    .00027    0 : qR1(5)3.5,2.5 : v=0  6  1 E 3.5 - v=0  5  1 E 2.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  39:<LineList>
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  7.5  E  2   6.5  E  2     9888.4330     9888.4346    -0.0016 1    .00059    0 : qR1(5)7.5,6.5 : v=0  6  1 E 7.5 - v=0  5  1 E 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  41:<LineList>
  8.5 A1  1   7.5 A2  1     9888.7310     9888.7260     0.0050 1    .00089    0 : qR0(5)8.5,7.5 : v=0  6  0 A1 8.5 - v=0  5  0 A2 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  42:<LineList>
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  4.5 A2  7   3.5 A1  6     9895.0260     9895.0343    -0.0083 1    4.1e-5    0 : qR3(5)4.5,3.5 : v=0  6  3 A2 4.5 - v=0  5  3 A1 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  44:<LineList>
  4.5 A1  7   3.5 A2  6     9895.0260     9895.0343    -0.0083 1    4.1e-5    0 : qR3(5)4.5,3.5 : v=0  6  3 A1 4.5 - v=0  5  3 A2 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  45:<LineList>
  7.5 A1  1   6.5 A2  1     9895.5080     9895.5050     0.0030 1    .00077    0 : qR0(5)7.5,6.5 : v=0  6  0 A1 7.5 - v=0  5  0 A2 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  46:<LineList>
  3.5  E 11   2.5  E  9     9907.0160     9907.0205    -0.0045 1    .00012    0 : qR2(5)3.5,2.5 : v=0  6  2 E 3.5 - v=0  5  2 E 2.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  47:<LineList>
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  5.5 A1  2   5.5 A2  2     9984.2030     9984.2155    -0.0125 1    7.8e-5    0 : qR0(5)5.5,5.5 : v=0  6  0 A1 5.5 - v=0  5  0 A2 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  51:<LineList>
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  7.5 A1  5   6.5 A2  6    11487.1980    11487.1948     0.0032 1    5.5e-5    0 : qR3(6)7.5,6.5 : v=0  7  3 A1 7.5 - v=0  6  3 A2 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  53:<LineList>
  6.5 A2  7   5.5 A1  7    11496.8200    11496.8336    -0.0136 1    4.7e-5    0 : qR3(6)6.5,5.5 : v=0  7  3 A2 6.5 - v=0  6  3 A1 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  54:<LineList>
  6.5 A1  7   5.5 A2  7    11496.8200    11496.8336    -0.0136 1    4.7e-5    0 : qR3(6)6.5,5.5 : v=0  7  3 A1 6.5 - v=0  6  3 A2 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  55:<LineList>
  8.5 A1  4   7.5 A2  5    11504.2090    11504.2007     0.0083 1    6.4e-5    0 : qR3(6)8.5,7.5 : v=0  7  3 A1 8.5 - v=0  6  3 A2 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  56:<LineList>
  8.5 A2  4   7.5 A1  4    11504.2090    11504.2007     0.0083 1    6.4e-5    0 : qR3(6)8.5,7.5 : v=0  7  3 A2 8.5 - v=0  6  3 A1 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  57:<LineList>
  6.5  E  9   5.5  E  9    11504.6560    11504.6533     0.0027 1    .00017    0 : qR2(6)6.5,5.5 : v=0  7  2 E 6.5 - v=0  6  2 E 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  58:<LineList>
  5.5 A2  3   4.5 A1  3    11504.8160    11504.8205    -0.0045 1    .00038    0 : qR0(6)5.5,4.5 : v=0  7  0 A2 5.5 - v=0  6  0 A1 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  59:<LineList>
  5.5  E  8   4.5  E  8    11507.2150    11507.2135     0.0015 1     .0003    0 : qR1(6)5.5,4.5 : v=0  7  1 E 5.5 - v=0  6  1 E 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  60:<LineList>
  7.5  E  7   6.5  E  7    11508.4630    11508.4551     0.0079 1     .0002    0 : qR2(6)7.5,6.5 : v=0  7  2 E 7.5 - v=0  6  2 E 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  61:<LineList>
  6.5  E  6   5.5  E  6    11509.2150    11509.2156    -0.0006 1    .00035    0 : qR1(6)6.5,5.5 : v=0  7  1 E 6.5 - v=0  6  1 E 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  62:<LineList>
  6.5 A2  2   5.5 A1  2    11510.7140    11510.7155    -0.0015 1    .00045    0 : qR0(6)6.5,5.5 : v=0  7  0 A2 6.5 - v=0  6  0 A1 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  63:<LineList>
  4.5  E 10   3.5  E  9    11520.8640    11520.8708    -0.0068 1    .00025    0 : qR1(6)4.5,3.5 : v=0  7  1 E 4.5 - v=0  6  1 E 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  64:<LineList>
  7.5  E  4   6.5  E  4    11521.0870    11521.0885    -0.0015 1    .00041    0 : qR1(6)7.5,6.5 : v=0  7  1 E 7.5 - v=0  6  1 E 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  65:<LineList>
  8.5  E  5   7.5  E  5    11522.6310    11522.6297     0.0013 1    .00023    0 : qR2(6)8.5,7.5 : v=0  7  2 E 8.5 - v=0  6  2 E 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  66:<LineList>
  7.5 A2  2   6.5 A1  2    11525.2790    11525.2780     0.0010 1    .00053    0 : qR0(6)7.5,6.5 : v=0  7  0 A2 7.5 - v=0  6  0 A1 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  67:<LineList>
  5.5 A1  8   4.5 A2  7    11526.9090    11526.9182    -0.0092 1      4e-5    0 : qR3(6)5.5,4.5 : v=0  7  3 A1 5.5 - v=0  6  3 A2 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  68:<LineList>
  5.5 A2  8   4.5 A1  7    11526.9090    11526.9182    -0.0092 1      4e-5    0 : qR3(6)5.5,4.5 : v=0  7  3 A2 5.5 - v=0  6  3 A1 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  69:<LineList>
  9.5 A2  1   8.5 A1  1    11533.0470    11533.0408     0.0062 1     .0007    0 : qR0(6)9.5,8.5 : v=0  7  0 A2 9.5 - v=0  6  0 A1 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  70:<LineList>
  8.5  E  2   7.5  E  2    11534.2890    11534.2826     0.0064 1    .00048    0 : qR1(6)8.5,7.5 : v=0  7  1 E 8.5 - v=0  6  1 E 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  71:<LineList>
  9.5  E  1   8.5  E  1    11536.8630    11536.8528     0.0102 1    .00055    0 : qR1(6)9.5,8.5 : v=0  7  1 E 9.5 - v=0  6  1 E 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  72:<LineList>
  8.5 A2  1   7.5 A1  1    11538.2740    11538.2708     0.0032 1    .00062    0 : qR0(6)8.5,7.5 : v=0  7  0 A2 8.5 - v=0  6  0 A1 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  73:<LineList>
  4.5  E 12   3.5  E 11    11540.3200    11540.3358    -0.0158 1    .00012    0 : qR2(6)4.5,3.5 : v=0  7  2 E 4.5 - v=0  6  2 E 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  74:<LineList>
  9.5  E  3   8.5  E  3    11548.1780    11548.1685     0.0095 1    .00026    0 : qR2(6)9.5,8.5 : v=0  7  2 E 9.5 - v=0  6  2 E 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  75:<LineList>
  9.5 A2  3   8.5 A1  3    11566.6410    11566.6381     0.0029 1    7.3e-5    0 : qR3(6)9.5,8.5 : v=0  7  3 A2 9.5 - v=0  6  3 A1 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  76:<LineList>
  9.5 A1  2   8.5 A2  3    11566.6410    11566.6381     0.0029 1    7.3e-5    0 : qR3(6)9.5,8.5 : v=0  7  3 A1 9.5 - v=0  6  3 A2 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  77:<LineList>
  4.5 A2  8   3.5 A1  7    11573.4720    11573.4833    -0.0113 1    3.4e-5    0 : qR3(6)4.5,3.5 : v=0  7  3 A2 4.5 - v=0  6  3 A1 3.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  78:<LineList>
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  8.5 A1  6   7.5 A2  6    13146.6720    13146.6706     0.0014 1    4.2e-5    0 : qR3(7)8.5,7.5 : v=0  8  3 A1 8.5 - v=0  7  3 A2 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  80:<LineList>
  8.5 A2  5   7.5 A1  5    13146.6720    13146.6706     0.0014 1    4.2e-5    0 : qR3(7)8.5,7.5 : v=0  8  3 A2 8.5 - v=0  7  3 A1 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  81:<LineList>
  7.5  E  8   6.5  E  9    13156.4970    13156.4994    -0.0024 1    .00013    0 : qR2(7)7.5,6.5 : v=0  8  2 E 7.5 - v=0  7  2 E 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  82:<LineList>
  6.5 A1  3   5.5 A2  3    13156.8820    13156.8866    -0.0046 1    .00029    0 : qR0(7)6.5,5.5 : v=0  8  0 A1 6.5 - v=0  7  0 A2 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  83:<LineList>
  6.5  E  8   5.5  E  8    13158.1600    13158.1637    -0.0037 1    .00023    0 : qR1(7)6.5,5.5 : v=0  8  1 E 6.5 - v=0  7  1 E 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  84:<LineList>
  7.5  E  6   6.5  E  6    13160.3720    13160.3730    -0.0010 1    .00027    0 : qR1(7)7.5,6.5 : v=0  8  1 E 7.5 - v=0  7  1 E 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  85:<LineList>
  9.5 A1  4   8.5 A2  4    13160.9770    13160.9721     0.0049 1    4.8e-5    0 : qR3(7)9.5,8.5 : v=0  8  3 A1 9.5 - v=0  7  3 A2 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  86:<LineList>
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  8.5  E  6   7.5  E  7    13161.1860    13161.1793     0.0067 1    .00015    0 : qR2(7)8.5,7.5 : v=0  8  2 E 8.5 - v=0  7  2 E 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  88:<LineList>
  7.5 A1  2   6.5 A2  2    13161.6490    13161.6527    -0.0037 1    .00034    0 : qR0(7)7.5,6.5 : v=0  8  0 A1 7.5 - v=0  7  0 A2 6.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  89:<LineList>
  6.5  E 10   5.5  E 11    13162.0150    13162.0223    -0.0073 1    .00011    0 : qR2(7)6.5,5.5 : v=0  8  2 E 6.5 - v=0  7  2 E 5.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  90:<LineList>
  5.5 A1  5   4.5 A2  3    13163.9770    13163.9811    -0.0041 1    .00025    0 : qR0(7)5.5,4.5 : v=0  8  0 A1 5.5 - v=0  7  0 A2 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  91:<LineList>
  5.5  E 10   4.5  E 10    13168.0730    13168.0824    -0.0094 1     .0002    0 : qR1(7)5.5,4.5 : v=0  8  1 E 5.5 - v=0  7  1 E 4.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  92:<LineList>
  8.5  E  4   7.5  E  4    13169.8500    13169.8491     0.0009 1     .0003    0 : qR1(7)8.5,7.5 : v=0  8  1 E 8.5 - v=0  7  1 E 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  93:<LineList>
  9.5  E  4   8.5  E  5    13172.5590    13172.5539     0.0051 1    .00016    0 : qR2(7)9.5,8.5 : v=0  8  2 E 9.5 - v=0  7  2 E 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  94:<LineList>
  8.5 A1  2   7.5 A2  2    13172.7380    13172.7328     0.0052 1    .00038    0 : qR0(7)8.5,7.5 : v=0  8  0 A1 8.5 - v=0  7  0 A2 7.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  95:<LineList>
 10.5 A1  1   9.5 A2  1    13178.0500    13178.0405     0.0095 1    .00049    0 : qR0(7)10.5,9.5 : v=0  8  0 A1 10.5 - v=0  7  0 A2 9.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  96:<LineList>
  9.5  E  2   8.5  E  2    13179.7520    13179.7529    -0.0009 1    .00035    0 : qR1(7)9.5,8.5 : v=0  8  1 E 9.5 - v=0  7  1 E 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  97:<LineList>
 10.5  E  1   9.5  E  1    13180.6590    13180.6496     0.0094 1    .00039    0 : qR1(7)10.5,9.5 : v=0  8  1 E 10.5 - v=0  7  1 E 9.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  98:<LineList>
  9.5 A1  1   8.5 A2  1    13182.1960    13182.1954     0.0006 1    .00044    0 : qR0(7)9.5,8.5 : v=0  8  0 A1 9.5 - v=0  7  0 A2 8.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   :  99:<LineList>
 10.5  E  2   9.5  E  3    13188.4280    13188.4208     0.0072 1    .00019    0 : qR2(7)10.5,9.5 : v=0  8  2 E 10.5 - v=0  7  2 E 9.5 : 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water-2 - 8X_1divCF3I_6dropsD2O_2barAr_150327_030611_with water.ovr   : 100:<LineList>
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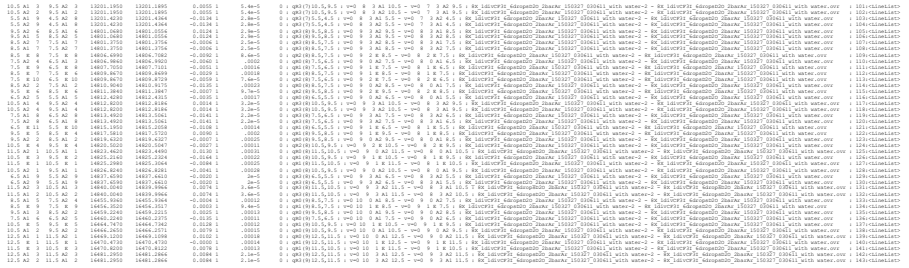

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143 Observations,  4 Parameters
Initial Average Error: 0.00736365520953737
Predicted New Error:   0.00736365520953097
Parameters:
  # Old                  New                  Std Dev    Change/Std Sens    Summary              Name
  1 823.299004985202     823.299004987023     .00013617     0.0000  1.24e-5 823.29900(14)        v=0 B
  2 .000138464032638431  .000138464042839527  9.2014e-7     0.0000  9e-8    1.3846(92)e-4        v=0 DJ
  3 .002070701486611839  .00207070149936434   1.0724e-5     0.0000  2.24e-6 2.071(11)e-3         v=0 DJK
  4 -2199.20785496269    -2199.2078550268     .04939776     0.0000  .014683 -2199.208(49)        Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.900   1.000
  3   0.368   0.064   1.000
  4  -0.089  -0.055  -0.063   1.000
```
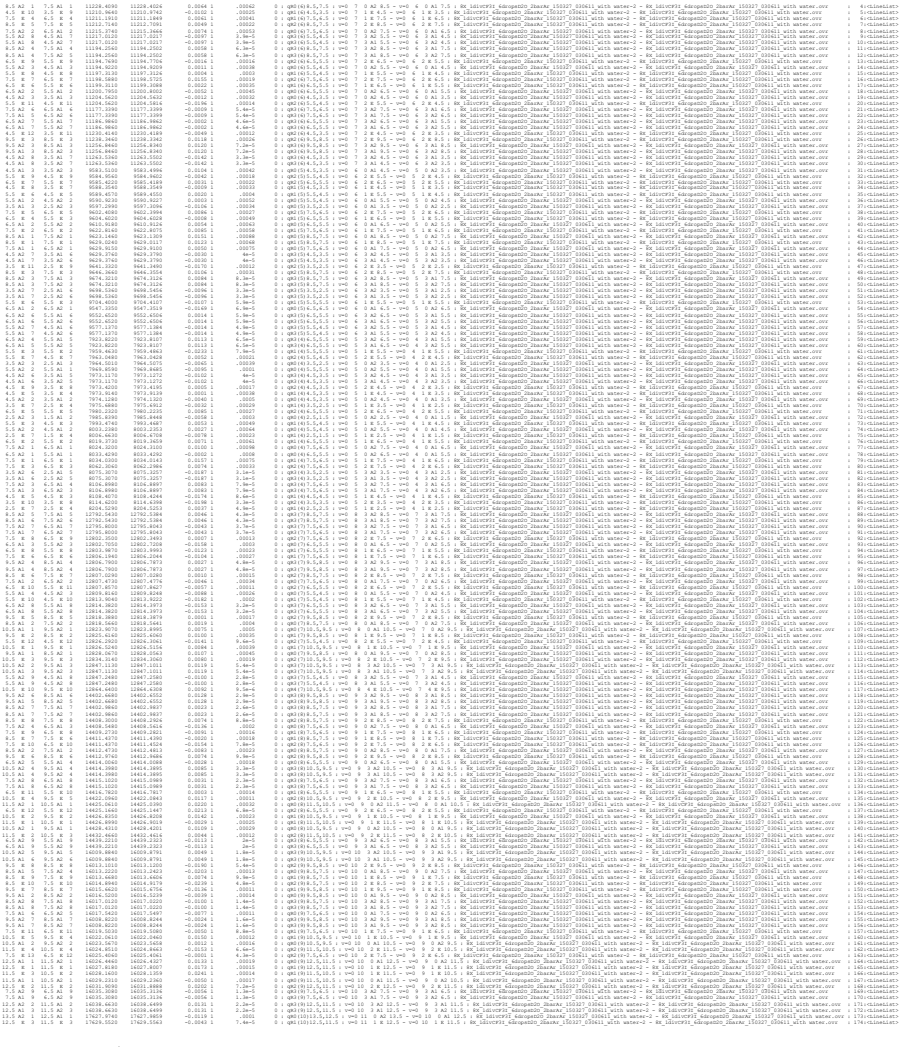

$D_2O\cdots ICF_3$, symmetric top, *m*=0 transitions

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_D2O_GROUND.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    SymmetricMolecule: SymmetricTop
      nNuclei         1
      JAdjustSym      False
      BlockMatrix     True
      PointGroup      C3v
      AlternateBasis False
      wt(A1,A2)       1
      wt(E)           1
      (Wt2)           1
      (Wt3)           1
      (Wt4)           1
      (Wt5)           1
      (Wt6)           1
      (Wt7)           1
      (Wt8)           1
      (Wt9)           1
      (Wt10)          1
      (Wt11)          1
      (Wt12)          1
      (Wt13)          1
      Abundance 1
      SymmetricManifold: Ground
        Initial        True
        Colour         Green
        EigenSearch    True
        LimitSearch    False
        AutoQConverge True
        UsePopParams   False
        SymmetricTop: v=0
          Symmetry A1
          Kmin     all
          Kmax     all
          B    801.163738027346           Float
          C    5600
          DJ  0.000133410321898007        Float
          DJK 0.00193663870271294         Float
          symmetricTopNucleus: Nucleus1
            Spin   2.5
            AsNext False
            eQq -2199.41601961075          Float
        <J,N,K,l|B|J,N,K,l> = N*(N+1)-K^2
        <J,N,K,l|C|J,N,K,l> = K^2
        <J,N,K,l|DJ|J,N,K,l> = -N^2*(N+1)^2
        <J,N,K,l|DJK|J,N,K,l> = -N*(N+1)*K^2
      TransitionMoments: <Ground|mu|Ground>
        CartesianTransitionMoment: <v=0|a|v=0>
          Axis a
          Strength 1
```



```
172 Observations,  4 Parameters
Initial Average Error: 0.0103338453206353
Predicted New Error:   0.0103338453206349
Parameters:
  # Old                  New                Std Dev    Change/Std Sens    Summary                Name
  1 801.163738027346     801.163738027893    .00016254     0.0000  1.68e-5 801.16374(16)          v=0 B
  2 .000133410321898007 .000133410325092375 1.0023e-6     0.0000  1.12e-7 1.334(10)e-4           v=0 DJ
  3 .00193663870271294   .00193663872439678 1.3108e-5     0.0000  2.86e-6 1.937(13)e-3           v=0 DJK
  4 -2199.41601961075    -2199.4160196109    .04999866     0.0000  .016341 -2199.416(50)          Nucleus1 eQq

Correlation Matrix
       1       2       3       4
  1   1.000
  2   0.881   1.000
  3   0.375   0.025   1.000
  4   0.009   0.041  -0.066   1.000
```

$H_2{}^{16}O\cdots ICF_3$, asymmetric top, K=0,1 transitions.

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_H2O_asym_K=0,1.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    AsymmetricMolecule: AsymmetricTop
      nNuclei         1
      JAdjustSym      False
      BlockMatrix     True
      PointGroup      C2v
      Representation Ir
```

```
SReduction     False
eeWt           1
eoWt           1
oeWt           1
ooWt           1
C2zAxis        a
C2xAxis        c
PseudoC2v      False
FakeSym        False
PhaseAdjust    False
Abundance 1
AsymmetricManifold: Ground
  Initial       True
  Colour        Red
  EigenSearch   True
  LimitSearch   True
  AutoQConverge True
  UsePopParams  False
  AsymmetricTop: Ground v=0
    Symmetry A1
    Kmin      2
    Kmax      2
    A       5600
    BBar   846.75774
    BDelta 1.95986
    DJK    -0.002183
    DJ     0.0001675
    AsymmetricTopNucleus: Ground Nucleus1
      Spin    2.5
      AsNext False
      CHIzz     -2199.03
      CHIxxmyy -19.71
  <J,N,K|A|J,N,K> = K^2
  <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
  <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
  <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
  <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
  <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
TransitionMoments: <Ground|mu|Ground>
  CartesianTransitionMoment: <Ground|mu|Ground> <v=0|a|v=0>
    Axis a
    Strength 1
AsymmetricManifold: Ground_K=0
  Initial       True
  Colour        Green
  EigenSearch   True
  LimitSearch   True
  AutoQConverge True
  UsePopParams  False
  AsymmetricTop: Ground_K=0 v=0
    Symmetry A1
    Kmin      0
    Kmax      1
    A       5600
    BBar   846.744956145439            Float
    BDelta 1.95944939942566            Float
    DJK    -0.0113550699773702         Float
    DJ     0.000131791812793793        Float
    AsymmetricTopNucleus: Ground_K=0 Nucleus1
      Spin    2.5
      AsNext False
      CHIzz     -2199.34387811855           Float
      CHIxxmyy -20.054692667688            Float
  <J,N,K|A|J,N,K> = K^2
  <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
  <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
  <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
  <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
  <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
TransitionMoments: <Ground_K=0|mu|Ground_K=0>
  CartesianTransitionMoment: <Ground_K=0|mu|Ground_K=0> <v=0|a|v=0>
    Axis a
    Strength 1
```

```
Residuals before fit for AsymmetricTop for the Ground_K=0 manifold
   J' S' #'    J" S" #"     Observed    Calculated     Obs-Calc  StdDev
  6.5 A1  1   5.5 A2  1    6792.3595    6792.3815     -0.0220 1    .00032    0 : qR0,3(3)6.5,5.5 : AsymmetricTop Ground_K=0 v=0  4  0  4 6.5 - Ground_K=0 v=0  3  0  3 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr :  1:<LineList>
  3.5 A2  3   2.5 A1  3    8420.3033    8420.3174     -0.0141 1    .00014    0 : qR0,4(4)3.5,2.5 : AsymmetricTop Ground_K=0 v=0  5  0  5 3.5 - Ground_K=0 v=0  4  0  4 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr :  2:<LineList>
  4.5 B1  4   3.5 B2  4    8424.9096    8424.9035      0.0061 1    .00029    0 : qR1,4(4)4.5,3.5 : Ground_K=0 v=0  5  1  5 4.5 - Ground_K=0 v=0  4  1  4 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               :  3:<LineList>
  3.5 B1  5   2.5 B2  4    8426.6227    8426.6143      0.0084 1    .00022    0 : qR1,4(4)3.5,2.5 : Ground_K=0 v=0  5  1  5 3.5 - Ground_K=0 v=0  4  1  4 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               :  4:<LineList>
  4.5 A2  2   3.5 A1  2    8430.0346    8430.0397     -0.0051 1    .00019    0 : qR0,4(4)4.5,3.5 : AsymmetricTop Ground_K=0 v=0  5  0  5 4.5 - Ground_K=0 v=0  4  0  4 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr :  5:<LineList>
  4.5 B2  4   3.5 B1  4    8434.9900    8434.9777      0.0123 1    .00029    0 : qR1,3(4)4.5,3.5 : Ground_K=0 v=0  5  1  4 4.5 - Ground_K=0 v=0  4  1  3 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               :  6:<LineList>
  3.5 B2  5   2.5 B1  4    8436.7969    8436.7908      0.0061 1    .00022    0 : qR1,3(4)3.5,2.5 : Ground_K=0 v=0  5  1  4 3.5 - Ground_K=0 v=0  4  1  3 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               :  7:<LineList>
  2.5 A2  3   1.5 A1  2    8441.6084    8441.6349     -0.0265 1    .00011    0 : qR0,4(4)2.5,1.5 : AsymmetricTop Ground_K=0 v=0  5  0  5 2.5 - Ground_K=0 v=0  4  0  4 1.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr :  8:<LineList>
  5.5 B1  3   4.5 B2  3    8444.5870    8444.5752      0.0118 1    .00037    0 : qR1,4(4)5.5,4.5 : Ground_K=0 v=0  5  1  5 5.5 - Ground_K=0 v=0  4  1  4 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               :  9:<LineList>
  5.5 B2  3   4.5 B1  3    8454.4183    8454.4080      0.0103 1    .00037    0 : qR1,3(4)5.5,4.5 : Ground_K=0 v=0  5  1  4 5.5 - Ground_K=0 v=0  4  1  3 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 10:<LineList>
  2.5 B1  5   1.5 B2  4    8457.6493    8457.6554     -0.0061 1    .00017    0 : qR1,4(4)2.5,1.5 : Ground_K=0 v=0  5  1  5 2.5 - Ground_K=0 v=0  4  1  4 1.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 11:<LineList>
  5.5 A2  2   4.5 A1  2    8459.2078    8459.2147     -0.0069 1    .00024    0 : qR0,4(4)5.5,4.5 : AsymmetricTop Ground_K=0 v=0  5  0  5 5.5 - Ground_K=0 v=0  4  0  4 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 12:<LineList>
  2.5 B2  5   1.5 B1  4    8467.6701    8467.6746     -0.0045 1    .00017    0 : qR1,3(4)2.5,1.5 : Ground_K=0 v=0  5  1  4 2.5 - Ground_K=0 v=0  4  1  3 1.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 13:<LineList>
  6.5 B1  2   5.5 B2  2    8470.6131    8470.6014      0.0117 1    .00047    0 : qR1,4(4)6.5,5.5 : Ground_K=0 v=0  5  1  5 6.5 - Ground_K=0 v=0  4  1  4 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 14:<LineList>
  7.5 A2  1   6.5 A1  1    8480.0349    8480.0553     -0.0204 1    .00037    0 : qR0,4(4)7.5,6.5 : AsymmetricTop Ground_K=0 v=0  5  0  5 7.5 - Ground_K=0 v=0  4  0  4 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 15:<LineList>
  6.5 B2  2   5.5 B1  2    8480.1912    8480.1854      0.0058 1    .00047    0 : qR1,3(4)6.5,5.5 : Ground_K=0 v=0  5  1  4 6.5 - Ground_K=0 v=0  4  1  3 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 16:<LineList>
  7.5 B1  1   6.5 B2  1    8485.0102    8485.0027      0.0075 1    .00057    0 : qR1,4(4)7.5,6.5 : Ground_K=0 v=0  5  1  5 7.5 - Ground_K=0 v=0  4  1  4 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 17:<LineList>
  6.5 A2  1   5.5 A1  1    8489.1690    8489.1835     -0.0145 1     .0003    0 : qR0,4(4)6.5,5.5 : AsymmetricTop Ground_K=0 v=0  5  0  5 6.5 - Ground_K=0 v=0  4  0  4 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 18:<LineList>
  7.5 B2  1   6.5 B1  1    8494.6907    8494.6821      0.0086 1    .00057    0 : qR1,3(4)7.5,6.5 : Ground_K=0 v=0  5  1  4 7.5 - Ground_K=0 v=0  4  1  3 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 19:<LineList>
  4.5 B2  5   3.5 B1  5   10129.5305   10129.5301      0.0004 1    .00024    0 : qR1,5(5)4.5,3.5 : Ground_K=0 v=0  6  1  6 4.5 - Ground_K=0 v=0  5  1  5 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 20:<LineList>
  4.5 A1  3   3.5 A2  3   10130.4880   10130.4943     -0.0063 1    .00018    0 : qR0,5(5)4.5,3.5 : AsymmetricTop Ground_K=0 v=0  6  0  6 4.5 - Ground_K=0 v=0  5  0  5 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 21:<LineList>
  5.5 B2  4   4.5 B1  4   10130.6844   10130.6812      0.0032 1     .0003    0 : qR1,5(5)5.5,4.5 : Ground_K=0 v=0  6  1  6 5.5 - Ground_K=0 v=0  5  1  5 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 22:<LineList>
  5.5 A1  2   4.5 A2  2   10137.9710   10137.9725     -0.0015 1    .00022    0 : qR0,5(5)5.5,4.5 : AsymmetricTop Ground_K=0 v=0  6  0  6 5.5 - Ground_K=0 v=0  5  0  5 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 23:<LineList>
  5.5 B1  4   4.5 B2  4   10142.6156   10142.6097      0.0059 1     .0003    0 : qR1,4(5)5.5,4.5 : Ground_K=0 v=0  6  1  5 5.5 - Ground_K=0 v=0  5  1  4 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 24:<LineList>
  3.5 A1  3   2.5 A2  3   10144.2614   10144.2796     -0.0182 1    .00015    0 : qR0,5(5)3.5,2.5 : AsymmetricTop Ground_K=0 v=0  6  0  6 3.5 - Ground_K=0 v=0  5  0  5 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 25:<LineList>
  6.5 B2  3   5.5 B1  3   10145.9145   10145.9114      0.0031 1    .00036    0 : qR1,5(5)6.5,5.5 : Ground_K=0 v=0  6  1  6 6.5 - Ground_K=0 v=0  5  1  5 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 26:<LineList>
  3.5 B2  6   2.5 B1  5   10149.3915   10149.4014     -0.0099 1     .0002    0 : qR1,5(5)3.5,2.5 : Ground_K=0 v=0  6  1  6 3.5 - Ground_K=0 v=0  5  1  5 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 27:<LineList>
  6.5 B1  3   5.5 B2  3   10157.6804   10157.6737      0.0067 1    .00036    0 : qR1,4(5)6.5,5.5 : Ground_K=0 v=0  6  1  5 6.5 - Ground_K=0 v=0  5  1  4 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 28:<LineList>
  6.5 A1  2   5.5 A2  2   10157.9705   10157.9746     -0.0041 1    .00027    0 : qR0,5(5)6.5,5.5 : AsymmetricTop Ground_K=0 v=0  6  0  6 6.5 - Ground_K=0 v=0  5  0  5 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 29:<LineList>
  3.5 B1  6   2.5 B2  5   10161.2885   10161.2969     -0.0084 1    .00016    0 : qR1,4(5)3.5,2.5 : Ground_K=0 v=0  6  1  5 3.5 - Ground_K=0 v=0  5  1  4 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 30:<LineList>
  7.5 B2  2   6.5 B1  2   10164.1679   10164.1618      0.0061 1    .00034    0 : qR1,5(5)7.5,6.5 : Ground_K=0 v=0  6  1  6 7.5 - Ground_K=0 v=0  5  1  5 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 31:<LineList>
  8.5 A1  1   7.5 A2  1   10170.0561   10170.0609     -0.0048 1    .00037    0 : qR0,5(5)8.5,7.5 : AsymmetricTop Ground_K=0 v=0  6  0  6 8.5 - Ground_K=0 v=0  5  0  5 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 32:<LineList>
  8.5 B2  1   7.5 B1  1   10170.2501   10170.2387      0.0114 1     .0005    0 : qR1,5(5)8.5,7.5 : Ground_K=0 v=0  6  1  6 8.5 - Ground_K=0 v=0  5  1  5 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 33:<LineList>
  7.5 B1  2   6.5 B2  2   10175.7713   10175.7662      0.0051 1    .00043    0 : qR1,4(5)7.5,6.5 : Ground_K=0 v=0  6  1  5 7.5 - Ground_K=0 v=0  5  1  4 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 34:<LineList>
  7.5 A1  1   6.5 A2  1   10176.8284   10176.8410     -0.0126 1    .00032    0 : qR0,5(5)7.5,6.5 : AsymmetricTop Ground_K=0 v=0  6  0  6 7.5 - Ground_K=0 v=0  5  0  5 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 35:<LineList>
  8.5 B1  1   7.5 B2  1   10181.9172   10181.9107      0.0065 1     .0005    0 : qR1,4(5)8.5,7.5 : Ground_K=0 v=0  6  1  5 8.5 - Ground_K=0 v=0  5  1  4 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 36:<LineList>
  5.5 B1  5   4.5 B2  5   11828.7208   11828.7237     -0.0029 1    .00021    0 : qR1,6(6)5.5,4.5 : Ground_K=0 v=0  7  1  7 5.5 - Ground_K=0 v=0  6  1  6 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 37:<LineList>
  6.5 B1  4   5.5 B2  4   11830.7661   11830.7592      0.0069 1    .00025    0 : qR1,6(6)6.5,5.5 : Ground_K=0 v=0  7  1  7 6.5 - Ground_K=0 v=0  6  1  6 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 38:<LineList>
  5.5 A2  3   4.5 A1  3   11833.0971   11833.0825      0.0146 1    .00019    0 : qR0,6(6)5.5,4.5 : AsymmetricTop Ground_K=0 v=0  7  0  7 5.5 - Ground_K=0 v=0  6  0  6 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 39:<LineList>
  6.5 A2  2   5.5 A1  2   11839.0140   11838.9939      0.0201 1    .00022    0 : qR0,6(6)6.5,5.5 : AsymmetricTop Ground_K=0 v=0  7  0  7 6.5 - Ground_K=0 v=0  6  0  6 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 40:<LineList>
  4.5 B1  6   3.5 B2  6   11842.4104   11842.4160     -0.0056 1    .00018    0 : qR1,6(6)4.5,3.5 : Ground_K=0 v=0  7  1  7 4.5 - Ground_K=0 v=0  6  1  6 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 41:<LineList>
  4.5 A2  3   3.5 A1  3   11842.7013   11842.7032     -0.0019 1    .00016    0 : qR0,6(6)4.5,3.5 : AsymmetricTop Ground_K=0 v=0  7  0  7 4.5 - Ground_K=0 v=0  6  0  6 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 42:<LineList>
  6.5 B2  4   5.5 B1  4   11844.5875   11844.5913     -0.0038 1    .00025    0 : qR1,5(6)6.5,5.5 : Ground_K=0 v=0  7  1  6 6.5 - Ground_K=0 v=0  6  1  5 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 43:<LineList>
  7.5 A2  2   6.5 A1  2   11853.5761   11853.5547      0.0214 1    .00026    0 : qR0,6(6)7.5,6.5 : AsymmetricTop Ground_K=0 v=0  7  0  7 7.5 - Ground_K=0 v=0  6  0  6 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 44:<LineList>
  8.5 B1  2   7.5 B2  2   11855.9230   11855.9223      0.0007 1    .00035    0 : qR1,6(6)8.5,7.5 : Ground_K=0 v=0  7  1  7 8.5 - Ground_K=0 v=0  6  1  6 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 45:<LineList>
  4.5 B2  6   3.5 B1  6   11856.2146   11856.2280     -0.0134 1    .00018    0 : qR1,5(6)4.5,3.5 : Ground_K=0 v=0  7  1  6 4.5 - Ground_K=0 v=0  6  1  5 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 46:<LineList>
  7.5 B2  3   6.5 B1  3   11856.4071   11856.4020      0.0051 1     .0003    0 : qR1,5(6)7.5,6.5 : Ground_K=0 v=0  7  1  6 7.5 - Ground_K=0 v=0  6  1  5 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 47:<LineList>
  9.5 B1  1   8.5 B2  1   11858.4460   11858.4438      0.0022 1    .00039    0 : qR1,6(6)9.5,8.5 : Ground_K=0 v=0  7  1  7 9.5 - Ground_K=0 v=0  6  1  6 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 48:<LineList>
  9.5 A2  1   8.5 A1  1   11861.2908   11861.2773      0.0135 1    .00035    0 : qR0,6(6)9.5,8.5 : AsymmetricTop Ground_K=0 v=0  7  0  7 9.5 - Ground_K=0 v=0  6  0  6 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 49:<LineList>
  8.5 A2  1   7.5 A1  1   11866.5234   11866.5066      0.0168 1     .0003    0 : qR0,6(6)8.5,7.5 : AsymmetricTop Ground_K=0 v=0  7  0  7 8.5 - Ground_K=0 v=0  6  0  6 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr : 50:<LineList>
  8.5 B2  2   7.5 B1  2   11869.5275   11869.5242      0.0033 1    .00034    0 : qR1,5(6)8.5,7.5 : Ground_K=0 v=0  7  1  6 8.5 - Ground_K=0 v=0  6  1  5 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 51:<LineList>
  9.5 B2  1   8.5 B1  1   11872.1049   11872.0962      0.0087 1    .00039    0 : qR1,5(6)9.5,8.5 : Ground_K=0 v=0  7  1  6 9.5 - Ground_K=0 v=0  6  1  5 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 52:<LineList>
  6.5 B2  5   5.5 B1  5   13525.6323   13525.6370     -0.0047 1    .00016    0 : qR1,7(7)6.5,5.5 : Ground_K=0 v=0  8  1  8 6.5 - Ground_K=0 v=0  7  1  7 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 53:<LineList>
  5.5 B2  6   4.5 B1  6   13535.5609   13535.5809     -0.0200 1    .00014    0 : qR1,7(7)5.5,4.5 : Ground_K=0 v=0  8  1  8 5.5 - Ground_K=0 v=0  7  1  7 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 54:<LineList>
  8.5 B2  3   7.5 B1  3   13537.3848   13537.3918     -0.0070 1    .00022    0 : qR1,7(7)8.5,7.5 : Ground_K=0 v=0  8  1  8 8.5 - Ground_K=0 v=0  7  1  7 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 55:<LineList>
  5.5 A1  3   4.5 A2  3   13539.1585   13539.1310      0.0275 1    .00018    0 : qR0,7(7)5.5,4.5 : Ground_K=0 v=0  8  0  8 5.5 - Ground_K=0 v=0  7  0  7 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 56:<LineList>
  6.5 B1  5   5.5 B2  5   13541.4286   13541.4385     -0.0099 1    .00016    0 : qR1,6(7)6.5,5.5 : Ground_K=0 v=0  8  1  7 6.5 - Ground_K=0 v=0  7  1  6 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 57:<LineList>
  7.5 B1  4   6.5 B2  4   13543.6239   13543.6309     -0.0070 1    .00019    0 : qR1,6(7)7.5,6.5 : Ground_K=0 v=0  8  1  7 7.5 - Ground_K=0 v=0  7  1  6 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 58:<LineList>
  9.5 B2  2   8.5 B1  2   13547.3145   13547.3195     -0.0050 1    .00024    0 : qR1,7(7)9.5,8.5 : Ground_K=0 v=0  8  1  8 9.5 - Ground_K=0 v=0  7  1  7 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 59:<LineList>
  5.5 B1  6   4.5 B2  6   13551.3102   13551.3269     -0.0167 1    .00014    0 : qR1,6(7)5.5,4.5 : Ground_K=0 v=0  8  1  7 5.5 - Ground_K=0 v=0  7  1  6 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 60:<LineList>
  9.5 B1  2   8.5 B2  2   13562.9012   13562.9061     -0.0049 1    .00024    0 : qR1,6(7)9.5,8.5 : Ground_K=0 v=0  8  1  7 9.5 - Ground_K=0 v=0  7  1  6 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr               : 61:<LineList>
 10.5 B1  1   9.5 B2  1   13563.8125   13563.8098      0.0027 1    .00027    0 : qR1,6(7)10.5,9.5 : Ground_K=0 v=0  8  1  7 10.5 - Ground_K=0 v=0  7  1  6 9.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr           : 62:<LineList>
```

```
62 Observations,  6 Parameters
Initial Average Error: 0.0117337943981785
Predicted New Error:   0.0117337943981768
Parameters:
  # Old               New                 Std Dev    Change/Std Sens    Summary            Name
  1 846.744956145439  846.7449561465      .00042881    0.0000  1.54e-5 846.74496(43)       Ground_K=0 v=0 BBar
```

```
  2 1.95944939942566    1.95944939967609    .0005795     0.0000  7.33e-5 1.95945(58)          Ground_K=0 v=0 BDelta
  3 -.0113550699773702  -.0113550699419102  .00026231    0.0000  1.83e-5 -0.01136(26)         Ground_K=0 v=0 DJK
  4 .000131791812793793 .000131791821641367 4.3659e-6    0.0000  1.63e-7 1.318(44)e-4         Ground_K=0 v=0 DJ
  5 -2199.34387811855   -2199.34387867505   .18767115    0.0000  .022804 -2199.34(19)         Ground_K=0 Nucleus1 CHIzz
  6 -20.054692667688    -20.054691768736    .48328495    0.0000  .061146 -20.05(48)           Ground_K=0 Nucleus1 CHIxxmyy

Correlation Matrix
       1       2       3       4       5       6
  1   1.000
  2   0.030   1.000
  3   0.261   0.007   1.000
  4   0.856   0.041  -0.187   1.000
  5  -0.274   0.028  -0.027  -0.181   1.000
  6  -0.003   0.256   0.036  -0.009  -0.029   1.000
```

$H_2{}^{16}O\cdots ICF_3$, asymmetric top, K=2 transitions.

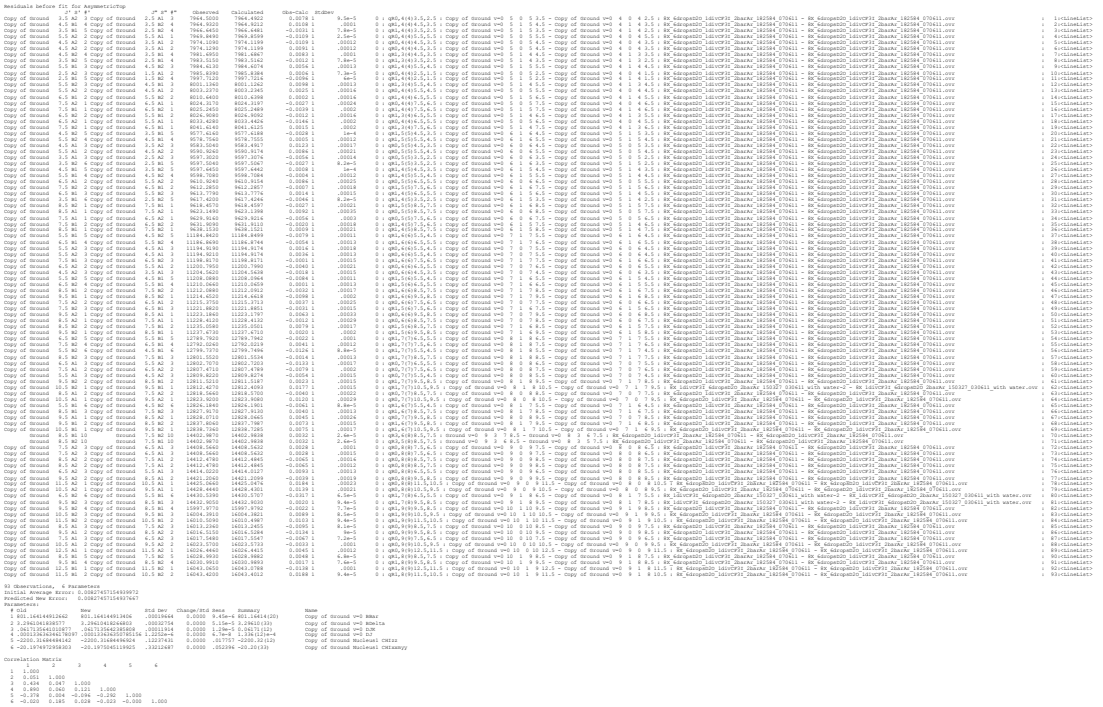
```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_H2O_sym_asym_K=2.pgo
  Units               MHz
  PrintLevel          Detail
  Precision           4
  BasisOrder          boDefault
  QuantumNumberFormat J
  FitCycles           1
  FitDetails          False
  AutoReplot          True
  AllowComplex        False
  NoLineList          False
  ShowEstUnc          False
  ShowDerivatives     False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    AsymmetricMolecule: AsymmetricTop
      nNuclei        1
      JAdjustSym     False
      BlockMatrix    True
      PointGroup     C2v
      Representation Ir
      SReduction     False
      eeWt           1
      eoWt           1
      oeWt           1
      ooWt           1
      C2zAxis        a
      C2xAxis        c
      PseudoC2v      False
      FakeSym        False
      PhaseAdjust    False
      Abundance 1
      AsymmetricManifold: Ground
        Initial       True
        Colour        Green
        EigenSearch   True
        LimitSearch   True
        AutoQConverge True
        UsePopParams  False
        AsymmetricTop: Ground v=0
          Symmetry A1
          Kmin     2
          Kmax     2
          A      5600
          BBar   846.74496
          BDelta 1.95986338170823
          DJK    -0.00629471666068682       Float
          DJ     0.00020931077215722        Float
          AsymmetricTopNucleus: Ground Nucleus1
            Spin   2.5
            AsNext False
            CHIzz    -2199.23326620246          Float
            CHIxxmyy -20.2
        <J,N,K|A|J,N,K> = K^2
        <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
        <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
        <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
        <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
        <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
      TransitionMoments: <Ground|mu|Ground>
        CartesianTransitionMoment: <Ground|mu|Ground> <v=0|a|v=0>
          Axis a
          Strength 1
      AsymmetricManifold: Copy of Ground
        Initial       True
        Colour        Red
        EigenSearch   True
        LimitSearch   True
        AutoQConverge True
        UsePopParams  False
        AsymmetricTop: Copy of Ground v=0
          Symmetry A1
          Kmin     0
          Kmax     1
          A      5600
          BBar   846.74496
          BDelta 1.95953319346395
          DJK    -0.01136
          DJ     0.0001318
          AsymmetricTopNucleus: Copy of Ground Nucleus1
```

```
            Spin   2.5
            AsNext False
            CHIzz    -2199.34
            CHIxxmyy -20.05
        <J,N,K|A|J,N,K> = K^2
        <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
        <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
        <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
        <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
        <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
      TransitionMoments: <Copy of Ground|mu|Copy of Ground>
        CartesianTransitionMoment: <Copy of Ground|mu|Copy of Ground> <v=0|a|v=0>
          Axis a
          Strength 1

Residuals before fit for AsymmetricTop for the Ground manifold
   J' S' #'    J" S" #"      Observed    Calculated      Obs-Calc  StdDev
  5.5 A2  3   4.5 A1  3     8419.0317     8419.0262      0.0055 1     .00011     0 : qR2,2(4)5.5,4.5 : Ground v=0  5  2  3 5.5 - Ground v=0  4  2  2 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   1:<LineList>
  5.5 A1  3   4.5 A2  3     8419.0317     8419.0262      0.0055 1     .00011     0 : qR2,3(4)5.5,4.5 : Ground v=0  5  2  4 5.5 - Ground v=0  4  2  3 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   2:<LineList>
  4.5 A2  4   3.5 A1  3     8429.5464     8429.5497     -0.0033 1     8.6e-5     0 : qR2,2(4)4.5,3.5 : Ground v=0  5  2  3 4.5 - Ground v=0  4  2  2 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   3:<LineList>
  4.5 A1  4   3.5 A2  3     8429.5464     8429.5497     -0.0033 1     8.6e-5     0 : qR2,3(4)4.5,3.5 : Ground v=0  5  2  4 4.5 - Ground v=0  4  2  3 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   4:<LineList>
  6.5 A1  2   5.5 A2  2     8436.6481     8436.6373      0.0108 1     .00014     0 : qR2,3(4)6.5,5.5 : Ground v=0  5  2  4 6.5 - Ground v=0  4  2  3 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   5:<LineList>
  6.5 A2  2   5.5 A1  2     8436.6481     8436.6373      0.0108 1     .00014     0 : qR2,2(4)6.5,5.5 : Ground v=0  5  2  3 6.5 - Ground v=0  4  2  2 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   6:<LineList>
  3.5 A1  4   2.5 A2  3     8467.1277     8467.1344     -0.0067 1     6.6e-5     0 : qR2,3(4)3.5,2.5 : Ground v=0  5  2  4 3.5 - Ground v=0  4  2  3 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   7:<LineList>
  3.5 A2  4   2.5 A1  3     8467.1277     8467.1344     -0.0067 1     6.6e-5     0 : qR2,2(4)3.5,2.5 : Ground v=0  5  2  3 3.5 - Ground v=0  4  2  2 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   8:<LineList>
  5.5 A1  4   4.5 A2  4    10132.2641    10132.2665     -0.0024 1     .00011     0 : qR2,3(5)5.5,4.5 : Ground v=0  6  2  4 5.5 - Ground v=0  5  2  3 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :   9:<LineList>
  5.5 A2  4   4.5 A1  4    10132.2641    10132.2665     -0.0024 1     .00011     0 : qR2,4(5)5.5,4.5 : Ground v=0  6  2  5 5.5 - Ground v=0  5  2  4 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  10:<LineList>
  6.5 A1  3   5.5 A2  3    10132.7031    10132.7005      0.0026 1     .00013     0 : qR2,3(5)6.5,5.5 : Ground v=0  6  2  4 6.5 - Ground v=0  5  2  3 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  11:<LineList>
  6.5 A2  3   5.5 A1  3    10132.7031    10132.7005      0.0026 1     .00013     0 : qR2,4(5)6.5,5.5 : Ground v=0  6  2  5 6.5 - Ground v=0  5  2  4 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  12:<LineList>
  7.5 A1  2   6.5 A2  2    10149.8715    10149.8658      0.0057 1     .00015     0 : qR2,3(5)7.5,6.5 : Ground v=0  6  2  4 7.5 - Ground v=0  5  2  3 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  13:<LineList>
  7.5 A2  2   6.5 A1  2    10149.8715    10149.8658      0.0057 1     .00015     0 : qR2,4(5)7.5,6.5 : Ground v=0  6  2  5 7.5 - Ground v=0  5  2  4 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  14:<LineList>
  4.5 A2  5   3.5 A1  4    10150.6575    10150.6637     -0.0062 1     8.7e-5     0 : qR2,4(5)4.5,3.5 : Ground v=0  6  2  5 4.5 - Ground v=0  5  2  4 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  15:<LineList>
  4.5 A1  5   3.5 A2  4    10150.6575    10150.6637     -0.0062 1     8.7e-5     0 : qR2,3(5)4.5,3.5 : Ground v=0  6  2  4 4.5 - Ground v=0  5  2  3 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  16:<LineList>
  3.5 A1  5   2.5 A2  4    10188.7610    10188.7746     -0.0136 1     7.1e-5     0 : qR2,3(5)3.5,2.5 : Ground v=0  6  2  4 3.5 - Ground v=0  5  2  3 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  17:<LineList>
  3.5 A2  5   2.5 A1  4    10188.7610    10188.7746     -0.0136 1     7.1e-5     0 : qR2,4(5)3.5,2.5 : Ground v=0  6  2  5 3.5 - Ground v=0  5  2  4 2.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  18:<LineList>
  8.5 A1  1   7.5 A2  1    10193.5326    10193.5245      0.0081 1     .00018     0 : qR2,3(5)8.5,7.5 : Ground v=0  6  2  4 8.5 - Ground v=0  5  2  3 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  19:<LineList>
  8.5 A2  1   7.5 A1  1    10193.5326    10193.5245      0.0081 1     .00018     0 : qR2,4(5)8.5,7.5 : Ground v=0  6  2  5 8.5 - Ground v=0  5  2  4 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  20:<LineList>
  7.5 A2  3   6.5 A1  3    11837.0671    11837.0712     -0.0041 1     .00013     0 : qR2,4(6)7.5,6.5 : Ground v=0  7  2  5 7.5 - Ground v=0  6  2  4 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  21:<LineList>
  7.5 A1  3   6.5 A2  3    11837.0671    11837.0712     -0.0041 1     .00013     0 : qR2,5(6)7.5,6.5 : Ground v=0  7  2  6 7.5 - Ground v=0  6  2  5 6.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  22:<LineList>
  5.5 A2  5   4.5 A1  5    11843.1130    11843.1205     -0.0075 1     9.4e-5     0 : qR2,4(6)5.5,4.5 : Ground v=0  7  2  5 5.5 - Ground v=0  6  2  4 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  23:<LineList>
  5.5 A1  5   4.5 A2  5    11843.1130    11843.1205     -0.0075 1     9.4e-5     0 : qR2,5(6)5.5,4.5 : Ground v=0  7  2  6 5.5 - Ground v=0  6  2  5 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  24:<LineList>
  8.5 A1  2   7.5 A2  2    11851.2884    11851.2851      0.0033 1     .00015     0 : qR2,5(6)8.5,7.5 : Ground v=0  7  2  6 8.5 - Ground v=0  6  2  5 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  25:<LineList>
  8.5 A2  2   7.5 A1  2    11851.2884    11851.2851      0.0033 1     .00015     0 : qR2,4(6)8.5,7.5 : Ground v=0  7  2  5 8.5 - Ground v=0  6  2  4 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  26:<LineList>
  4.5 A2  6   3.5 A1  5    11868.9834    11868.9896     -0.0062 1     7.9e-5     0 : qR2,4(6)4.5,3.5 : Ground v=0  7  2  5 4.5 - Ground v=0  6  2  4 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  27:<LineList>
  4.5 A1  6   3.5 A2  5    11868.9834    11868.9896     -0.0062 1     7.9e-5     0 : qR2,5(6)4.5,3.5 : Ground v=0  7  2  6 4.5 - Ground v=0  6  2  5 3.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  28:<LineList>
  9.5 A1  1   8.5 A2  1    11876.7526    11876.7407      0.0119 1     .00017     0 : qR2,5(6)9.5,8.5 : Ground v=0  7  2  6 9.5 - Ground v=0  6  2  5 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  29:<LineList>
  9.5 A2  1   8.5 A1  1    11876.7526    11876.7407      0.0119 1     .00017     0 : qR2,4(6)9.5,8.5 : Ground v=0  7  2  5 9.5 - Ground v=0  6  2  4 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  30:<LineList>
  8.5 A1  3   7.5 A2  3    13536.7084    13536.7097     -0.0013 1     .00012     0 : qR2,5(7)8.5,7.5 : Ground v=0  8  2  6 8.5 - Ground v=0  7  2  5 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  31:<LineList>
  8.5 A2  3   7.5 A1  3    13536.7084    13536.7097     -0.0013 1     .00012     0 : qR2,6(7)8.5,7.5 : Ground v=0  8  2  7 8.5 - Ground v=0  7  2  6 7.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  32:<LineList>
  6.5 A1  5   5.5 A2  5    13537.5553    13537.5610     -0.0057 1     8.8e-5     0 : qR2,5(7)6.5,5.5 : Ground v=0  8  2  6 6.5 - Ground v=0  7  2  5 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  33:<LineList>
  6.5 A2  5   5.5 A1  5    13537.5553    13537.5610     -0.0057 1     8.8e-5     0 : qR2,6(7)6.5,5.5 : Ground v=0  8  2  7 6.5 - Ground v=0  7  2  6 5.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  34:<LineList>
  9.5 A2  2   8.5 A1  2    13548.1036    13548.1001      0.0035 1     .00013     0 : qR2,6(7)9.5,8.5 : Ground v=0  8  2  7 9.5 - Ground v=0  7  2  6 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  35:<LineList>
  9.5 A1  2   8.5 A2  2    13548.1036    13548.1001      0.0035 1     .00013     0 : qR2,5(7)9.5,8.5 : Ground v=0  8  2  6 9.5 - Ground v=0  7  2  5 8.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  36:<LineList>
  5.5 A1  6   4.5 A2  6    13556.0224    13556.0270     -0.0046 1     7.7e-5     0 : qR2,5(7)5.5,4.5 : Ground v=0  8  2  6 5.5 - Ground v=0  7  2  5 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  37:<LineList>
  5.5 A2  6   4.5 A1  6    13556.0224    13556.0270     -0.0046 1     7.7e-5     0 : qR2,6(7)5.5,4.5 : Ground v=0  8  2  7 5.5 - Ground v=0  7  2  6 4.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  38:<LineList>
 10.5 A1  1   9.5 A2  1    13563.9283    13563.9175      0.0108 1     .00015     0 : qR2,5(7)10.5,9.5 : Ground v=0  8  2  6 10.5 - Ground v=0  7  2  5 9.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  39:<LineList>
 10.5 A2  1   9.5 A1  1    13563.9283    13563.9175      0.0108 1     .00015     0 : qR2,6(7)10.5,9.5 : Ground v=0  8  2  7 10.5 - Ground v=0  7  2  6 9.5 : 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411 - 4X_alone_3dropsH2O_1divCF3I_balance1-112barAr_89264shots_120411.ovr  :  40:<LineList>

40 Observations,  3 Parameters
Initial Average Error: 0.00729398083941763
Predicted New Error:   0.00729398083941695
Parameters:
  # Old                 New                  Std Dev   Change/Std Sens    Summary            Name
  1 -.00629471666068682 -.00629471642681538 8.9386e-5    0.0000  4.58e-6 -6.295(89)e-3       Ground v=0 DJK
  2 .00020931077215722  .000209310763106338 3.4677e-6    0.0000  1.82e-7 2.093(35)e-4        Ground v=0 DJ
  3 -2199.23326620246   -2199.23326605926   .12444202    0.0000  .023252 -2199.23(12)        Ground Nucleus1 CHIzz

Correlation Matrix
       1       2       3
  1   1.000
  2  -0.968   1.000
  3   0.450  -0.409   1.000
```

$D_2{}^{16}O\cdots ICF_3$, asymmetric top, K=0,1 transitions

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_D2O_sym_asym_K=0,1.pgo
  Units               MHz
  PrintLevel          Detail
  Precision           4
  BasisOrder          boDefault
  QuantumNumberFormat J
  FitCycles           1
  FitDetails          False
  AutoReplot          True
  AllowComplex        False
  NoLineList          False
  ShowEstUnc          False
  ShowDerivatives     False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    AsymmetricMolecule: AsymmetricTop
      nNuclei        1
      JAdjustSym     False
      BlockMatrix    True
      PointGroup     C2v
      Representation Ir
      SReduction     False
      eeWt           1
      eoWt           1
      oeWt           1
      ooWt           1
      C2zAxis        a
      C2xAxis        c
      PseudoC2v      False
      FakeSym        False
      PhaseAdjust    False
      Abundance 1
      AsymmetricManifold: Ground
        Initial      True
        Colour       Red
        EigenSearch  True
        LimitSearch  True
        AutoQConverge True
        UsePopParams  False
        AsymmetricTop: Ground v=0
          Symmetry A1
          Kmin     0
          Kmax     3
          A    5600
          BBar 801.163738
          DJK  0.001936638
          DJ   0.0001334
          AsymmetricTopNucleus: Ground Nucleus1
            Spin    2.5
            AsNext False
```

```
        CHIzz -2199.41602
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <Ground|mu|Ground>
    CartesianTransitionMoment: <Ground|mu|Ground> <v=0|a|v=0>
      Axis a
      Strength 1
  AsymmetricManifold: Copy of Ground
    Initial        True
    Colour         Blue
    EigenSearch    True
    LimitSearch    True
    AutoQConverge  True
    UsePopParams   False
    AsymmetricTop: Copy of Ground v=0
      Symmetry A1
      Kmin     0
      Kmax     1
      A       5600
      BBar    801.1641449126662           Float
      BDelta 3.2961041838577              Float
      DJK     0.0617135641010877          Float
      DJ      0.000133636346178097        Float
      AsymmetricTopNucleus: Copy of Ground Nucleus1
        Spin   2.5
        AsNext False
        CHIzz    -2200.31684484142          Float
        CHIxxmyy -20.1974972958303          Float
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
    <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <Copy of Ground|mu|Copy of Ground>
    CartesianTransitionMoment: <Copy of Ground|mu|Copy of Ground> <v=0|a|v=0>
      Axis a
      Strength 1
```



$D_2{}^{16}O\cdots ICF_3$, asymmetric top, K=2 transitions

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_D2O_sym_asym_K=2only.pgo
  Units                MHz
  PrintLevel           Detail
  Precision            4
  BasisOrder           boDefault
  QuantumNumberFormat  J
  FitCycles            1
  FitDetails           False
  AutoReplot           True
  AllowComplex         False
  NoLineList           False
  ShowEstUnc           False
  ShowDerivatives      False
  SVDThresh    1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
```

```
Concentration 1
AsymmetricMolecule: AsymmetricTop
  nNuclei         1
  JAdjustSym      False
  BlockMatrix     True
  PointGroup      C2v
  Representation  Ir
  SReduction      False
  eeWt            1
  eoWt            1
  oeWt            1
  ooWt            1
  C2zAxis         a
  C2xAxis         c
  PseudoC2v       False
  FakeSym         False
  PhaseAdjust     False
  Abundance 1
  AsymmetricManifold: Ground
    Initial       True
    Colour        Red
    EigenSearch   True
    LimitSearch   True
    AutoQConverge True
    UsePopParams  False
    AsymmetricTop: Ground v=0
      Symmetry A1
      Kmin     1
      Kmax     3
      A    5600
      BBar 801.163738
      DJK  0.001936638
      DJ   0.0001334
      AsymmetricTopNucleus: Ground Nucleus1
        Spin   2.5
        AsNext False
        CHIzz -2199.41602
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <Ground|mu|Ground>
    CartesianTransitionMoment: <Ground|mu|Ground> <v=0|a|v=0>
      Axis a
      Strength 1
  AsymmetricManifold: Copy of Ground
    Initial       True
    Colour        Red
    EigenSearch   True
    LimitSearch   True
    AutoQConverge True
    UsePopParams  False
    AsymmetricTop: Copy of Ground v=0
      Symmetry A1
      Kmin     0
      Kmax     1
      A      5600
      BBar   801.164400840379
      BDelta 3.29645468249942
      DJK    0.0617698564277422
      DJ     0.000134992923232828
      AsymmetricTopNucleus: Copy of Ground Nucleus1
        Spin   2.5
        AsNext False
        CHIzz    -2200.35839761593
        CHIxxmyy -20.1779861126728
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
    <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <Copy of Ground|mu|Copy of Ground>
    CartesianTransitionMoment: <Copy of Ground|mu|Copy of Ground> <v=0|a|v=0>
      Axis a
      Strength 1
  AsymmetricManifold: K=2
    Initial       True
    Colour        Blue
    EigenSearch   True
    LimitSearch   True
    AutoQConverge True
    UsePopParams  False
    AsymmetricTop: K=2 v=0
      Symmetry A1
      Kmin     2
      Kmax     2
      A      5600
      BBar   801.164400840379
      BDelta 3.29642566712775
      DJK    0.0121071586639545         Float
      DJ     0.000344043780893732       Float
      AsymmetricTopNucleus: K=2 Nucleus1
        Spin   2.5
        AsNext False
        CHIzz    -2200.51125950873          Float
        CHIxxmyy -20.2553395205889
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
    <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
```

```
        <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
      TransitionMoments: <K=2|mu|K=2>
        CartesianTransitionMoment: <K=2|mu|K=2> <v=0|a|v=0>
          Axis a
          Strength 1
```

Residuals before fit for AsymmetricTop for the K=2 manifold

```
  J' S' #'   J" S" #"    Observed    Calculated    Obs-Calc  StdDev
5.5 A2 3  4.5 A1 3  7962.5150  7962.5144  0.0006 1  6.1e-5  0 : qR2,2(4)5.5,4.5 : K=2 v=0 5 2 3 5.5 - K=2 v=0 4 2 2 4.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 1:<LineList>
5.5 A1 3  4.5 A2 3  7962.5150  7962.5144  0.0006 1  6.1e-5  0 : qR2,3(4)5.5,4.5 : K=2 v=0 5 2 4 5.5 - K=2 v=0 4 2 3 4.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 2:<LineList>
6.5 A2 2  5.5 A1 2  7979.7110  7979.6992  0.0118 1  7.7e-5  0 : qR2,2(4)6.5,5.5 : K=2 v=0 5 2 3 6.5 - K=2 v=0 4 2 2 5.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 3:<LineList>
6.5 A1 2  5.5 A2 2  7979.7110  7979.6992  0.0118 1  7.7e-5  0 : qR2,3(4)6.5,5.5 : K=2 v=0 5 2 4 6.5 - K=2 v=0 4 2 3 5.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 4:<LineList>
3.5 A2 4  2.5 A1 3  8010.3170  8010.3220  -0.0050 1  3.7e-5  0 : qR2,2(4)3.5,2.5 : K=2 v=0 5 2 3 3.5 - K=2 v=0 4 2 2 2.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 5:<LineList>
3.5 A1 4  2.5 A2 3  8010.3170  8010.3220  -0.0050 1  3.7e-5  0 : qR2,3(4)3.5,2.5 : K=2 v=0 5 2 4 3.5 - K=2 v=0 4 2 3 2.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 6:<LineList>
7.5 A2 1  6.5 A1 1  8061.8100  8061.8206  -0.0106 1  9.4e-5  0 : qR2,2(4)7.5,6.5 : K=2 v=0 5 2 3 7.5 - K=2 v=0 4 2 2 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 7:<LineList>
7.5 A1 1  6.5 A2 1  8061.8100  8061.8206  -0.0106 1  9.4e-5  0 : qR2,3(4)7.5,6.5 : K=2 v=0 5 2 4 7.5 - K=2 v=0 4 2 3 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 8:<LineList>
5.5 A2 4  4.5 A1 4  9584.2780  9584.2837  -0.0057 1  6e-5  0 : qR2,4(5)5.5,4.5 : K=2 v=0 6 2 5 5.5 - K=2 v=0 5 2 4 4.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 9:<LineList>
5.5 A1 4  4.5 A2 4  9584.2780  9584.2837  -0.0057 1  6e-5  0 : qR2,3(5)5.5,4.5 : K=2 v=0 6 2 4 5.5 - K=2 v=0 5 2 3 4.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 10:<LineList>
6.5 A2 3  5.5 A1 3  9584.7480  9584.7428  0.0052 1  7.3e-5  0 : qR2,4(5)6.5,5.5 : K=2 v=0 6 2 5 6.5 - K=2 v=0 5 2 4 5.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 11:<LineList>
6.5 A1 3  5.5 A2 3  9584.7480  9584.7428  0.0052 1  7.3e-5  0 : qR2,3(5)6.5,5.5 : K=2 v=0 6 2 4 6.5 - K=2 v=0 5 2 3 5.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 12:<LineList>
7.5 A1 2  6.5 A2 2  9601.7350  9601.7299  0.0051 1  8.7e-5  0 : qR2,3(5)7.5,6.5 : K=2 v=0 6 2 4 7.5 - K=2 v=0 5 2 3 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 13:<LineList>
7.5 A2 2  6.5 A1 2  9601.7350  9601.7299  0.0051 1  8.7e-5  0 : qR2,4(5)7.5,6.5 : K=2 v=0 6 2 5 7.5 - K=2 v=0 5 2 4 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 14:<LineList>
4.5 A2 5  3.5 A1 4  9602.5960  9602.6036  -0.0076 1  4.9e-5  0 : qR2,4(5)4.5,3.5 : K=2 v=0 6 2 5 4.5 - K=2 v=0 5 2 4 3.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 15:<LineList>
4.5 A1 5  3.5 A2 4  9602.5960  9602.6036  -0.0076 1  4.9e-5  0 : qR2,3(5)4.5,3.5 : K=2 v=0 6 2 4 4.5 - K=2 v=0 5 2 3 3.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 16:<LineList>
3.5 A2 5  2.5 A1 4  9640.6880  9640.6992  -0.0112 1  4e-5  0 : qR2,4(5)3.5,2.5 : K=2 v=0 6 2 5 3.5 - K=2 v=0 5 2 4 2.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 17:<LineList>
3.5 A1 5  2.5 A2 4  9640.6880  9640.6992  -0.0112 1  4e-5  0 : qR2,3(5)3.5,2.5 : K=2 v=0 6 2 4 3.5 - K=2 v=0 5 2 3 2.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 18:<LineList>
8.5 A1 1  7.5 A2 1  9645.7110  9645.7107  0.0003 1  .0001  0 : qR2,3(5)8.5,7.5 : K=2 v=0 6 2 4 8.5 - K=2 v=0 5 2 3 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 19:<LineList>
8.5 A2 1  7.5 A1 1  9645.7110  9645.7107  0.0003 1  .0001  0 : qR2,4(5)8.5,7.5 : K=2 v=0 6 2 5 8.5 - K=2 v=0 5 2 4 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 20:<LineList>
7.5 A2 3  6.5 A1 3  11197.7120  11197.7146  -0.0026 1  7.5e-5  0 : qR2,4(6)7.5,6.5 : K=2 v=0 7 2 5 7.5 - K=2 v=0 6 2 4 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 21:<LineList>
7.5 A1 3  6.5 A2 3  11197.7120  11197.7146  -0.0026 1  7.5e-5  0 : qR2,5(6)7.5,6.5 : K=2 v=0 7 2 6 7.5 - K=2 v=0 6 2 5 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 22:<LineList>
5.5 A2 5  4.5 A1 5  11203.7150  11203.7263  -0.0113 1  5.4e-5  0 : qR2,4(6)5.5,4.5 : K=2 v=0 7 2 5 5.5 - K=2 v=0 6 2 4 4.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 23:<LineList>
5.5 A1 5  4.5 A2 5  11203.7150  11203.7263  -0.0113 1  5.4e-5  0 : qR2,5(6)5.5,4.5 : K=2 v=0 7 2 6 5.5 - K=2 v=0 6 2 5 4.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 24:<LineList>
8.5 A1 2  7.5 A2 2  11211.8590  11211.8573  0.0017 1  8.7e-5  0 : qR2,5(6)8.5,7.5 : K=2 v=0 7 2 6 8.5 - K=2 v=0 6 2 5 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 25:<LineList>
8.5 A2 2  7.5 A1 2  11211.8590  11211.8573  0.0017 1  8.7e-5  0 : qR2,4(6)8.5,7.5 : K=2 v=0 7 2 5 8.5 - K=2 v=0 6 2 4 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 26:<LineList>
4.5 A2 6  3.5 A1 5  11229.5740  11229.5760  -0.0020 1  4.6e-5  0 : qR2,4(6)4.5,3.5 : K=2 v=0 7 2 5 4.5 - K=2 v=0 6 2 4 3.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 27:<LineList>
4.5 A1 6  3.5 A2 5  11229.5740  11229.5760  -0.0020 1  4.6e-5  0 : qR2,5(6)4.5,3.5 : K=2 v=0 7 2 6 4.5 - K=2 v=0 6 2 5 3.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 28:<LineList>
9.5 A2 1  8.5 A1 1  11237.5050  11237.4969  0.0081 1  1e-4  0 : qR2,4(6)9.5,8.5 : K=2 v=0 7 2 5 9.5 - K=2 v=0 6 2 4 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 29:<LineList>
9.5 A1 1  8.5 A2 1  11237.5050  11237.4969  0.0081 1  1e-4  0 : qR2,5(6)9.5,8.5 : K=2 v=0 7 2 6 9.5 - K=2 v=0 6 2 5 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 30:<LineList>
7.5 A2 4  6.5 A1 4  12801.2640  12801.2696  -0.0056 1  6e-5  0 : qR2,6(7)7.5,6.5 : K=2 v=0 8 2 7 7.5 - K=2 v=0 7 2 6 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 31:<LineList>
7.5 A1 4  6.5 A2 4  12801.2640  12801.2696  -0.0056 1  6e-5  0 : qR2,5(7)7.5,6.5 : K=2 v=0 8 2 6 7.5 - K=2 v=0 7 2 5 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 32:<LineList>
8.5 A2 3  7.5 A1 3  12805.9500  12805.9506  -0.0006 1  6.9e-5  0 : qR2,6(7)8.5,7.5 : K=2 v=0 8 2 7 8.5 - K=2 v=0 7 2 6 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 33:<LineList>
8.5 A1 3  7.5 A2 3  12805.9500  12805.9506  -0.0006 1  6.9e-5  0 : qR2,5(7)8.5,7.5 : K=2 v=0 8 2 6 8.5 - K=2 v=0 7 2 5 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 34:<LineList>
9.5 A1 2  8.5 A2 2  12817.3210  12817.3159  0.0051 1  7.8e-5  0 : qR2,5(7)9.5,8.5 : K=2 v=0 8 2 6 9.5 - K=2 v=0 7 2 5 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 35:<LineList>
9.5 A2 2  8.5 A1 2  12817.3210  12817.3159  0.0051 1  7.8e-5  0 : qR2,6(7)9.5,8.5 : K=2 v=0 8 2 7 9.5 - K=2 v=0 7 2 6 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 36:<LineList>
10.5 A2 1  9.5 A1 1  12833.2630  12833.2429  0.0201 1  8.8e-5  0 : qR2,6(7)10.5,9.5 : K=2 v=0 8 2 7 10.5 - K=2 v=0 7 2 6 9.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 37:<LineList>
10.5 A1 1  9.5 A2 1  12833.2630  12833.2429  0.0201 1  8.8e-5  0 : qR2,5(7)10.5,9.5 : K=2 v=0 8 2 6 10.5 - K=2 v=0 7 2 5 9.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 38:<LineList>
8.5 A2 4  7.5 A1 4  14406.9390  14406.9519  -0.0129 1  5.1e-5  0 : qR2,6(8)8.5,7.5 : K=2 v=0 9 2 7 8.5 - K=2 v=0 8 2 6 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 39:<LineList>
8.5 A1 4  7.5 A2 4  14406.9390  14406.9519  -0.0129 1  5.1e-5  0 : qR2,7(8)8.5,7.5 : K=2 v=0 9 2 8 8.5 - K=2 v=0 8 2 7 7.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 40:<LineList>
7.5 A2 5  6.5 A1 5  14410.1240  14410.1132  0.0108 1  4.5e-5  0 : qR2,6(8)7.5,6.5 : K=2 v=0 9 2 7 7.5 - K=2 v=0 8 2 6 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 41:<LineList>
7.5 A1 5  6.5 A2 5  14410.1240  14410.1132  0.0108 1  4.5e-5  0 : qR2,7(8)7.5,6.5 : K=2 v=0 9 2 8 7.5 - K=2 v=0 8 2 7 6.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 42:<LineList>
9.5 A2 3  8.5 A1 3  14411.6280  14411.6302  -0.0022 1  5.8e-5  0 : qR2,6(8)9.5,8.5 : K=2 v=0 9 2 7 9.5 - K=2 v=0 8 2 6 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 43:<LineList>
9.5 A1 3  8.5 A2 3  14411.6280  14411.6302  -0.0022 1  5.8e-5  0 : qR2,7(8)9.5,8.5 : K=2 v=0 9 2 8 9.5 - K=2 v=0 8 2 7 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 44:<LineList>
6.5 A2 6  5.5 A1 6  14423.8170  14423.8122  0.0048 1  4e-5  0 : qR2,6(8)6.5,5.5 : K=2 v=0 9 2 7 6.5 - K=2 v=0 8 2 6 5.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 45:<LineList>
6.5 A1 6  5.5 A2 6  14423.8170  14423.8122  0.0048 1  4e-5  0 : qR2,7(8)6.5,5.5 : K=2 v=0 9 2 8 6.5 - K=2 v=0 8 2 7 5.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 46:<LineList>
11.5 A2 1  10.5 A1 1  14431.1520  14431.1334  0.0186 1  7.2e-5  0 : qR2,6(8)11.5,10.5 : K=2 v=0 9 2 7 11.5 - K=2 v=0 8 2 6 10.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 47:<LineList>
11.5 A1 1  10.5 A2 1  14431.1520  14431.1334  0.0186 1  7.2e-5  0 : qR2,7(8)11.5,10.5 : K=2 v=0 9 2 8 11.5 - K=2 v=0 8 2 7 10.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 48:<LineList>
9.5 A2 4  8.5 A1 4  16011.4650  16011.4723  -0.0073 1  4e-5  0 : qR2,8(9)9.5,8.5 : K=2 v=0 10 2 9 9.5 - K=2 v=0 9 2 8 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 49:<LineList>
9.5 A1 4  8.5 A2 4  16011.4650  16011.4723  -0.0073 1  4e-5  0 : qR2,7(9)9.5,8.5 : K=2 v=0 10 2 8 9.5 - K=2 v=0 9 2 7 8.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 50:<LineList>
10.5 A2 3  9.5 A1 3  16015.8260  16015.8394  -0.0134 1  4.4e-5  0 : qR2,8(9)10.5,9.5 : K=2 v=0 10 2 9 10.5 - K=2 v=0 9 2 8 9.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 51:<LineList>
10.5 A1 3  9.5 A2 3  16015.8260  16015.8394  -0.0134 1  4.4e-5  0 : qR2,7(9)10.5,9.5 : K=2 v=0 10 2 8 10.5 - K=2 v=0 9 2 7 9.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 52:<LineList>
11.5 A2 2  10.5 A1 2  16023.2270  16023.2244  0.0026 1  4.9e-5  0 : qR2,8(9)11.5,10.5 : K=2 v=0 10 2 9 11.5 - K=2 v=0 9 2 8 10.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 53:<LineList>
11.5 A1 2  10.5 A2 2  16023.2270  16023.2244  0.0026 1  4.9e-5  0 : qR2,7(9)11.5,10.5 : K=2 v=0 10 2 8 11.5 - K=2 v=0 9 2 7 10.5 : 8X_6dropsD2O_1divCF3I_2barAr_182584_070611 - 8X_6dropsD2O_1divCF3I_2barAr_182584_070611.ovr : 54:<LineList>
```

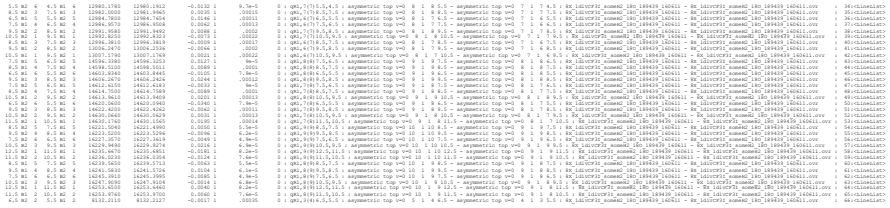
```
54 Observations,  3 Parameters
Initial Average Error: 0.00910157158477699
Predicted New Error:   0.0091015715847767
Parameters:
  # Old                   New                   Std Dev    Change/Std Sens     Summary              Name
  1 .01210715866639544    .012107158772757      6.1296e-5    0.0000  5.05e-6 0.012107(61)         K=2 v=0 DJK
  2 .000344043780893732 .000344043778262581 1.7254e-6    0.0000  1.43e-7 3.440(17)e-4         K=2 v=0 DJ
  3 -2200.51125950873    -2200.51125948772    .12624518    0.0000  .030592 -2200.51(13)         K=2 Nucleus1 CHIzz

Correlation Matrix
       1       2       3
  1   1.000
  2  -0.941   1.000
  3   0.093  -0.049   1.000
```

$H_2{}^{18}O\cdots ICF_3$, asymmetric top, K=1 transitions

```
Pgopher 7.1.187 04 Apr 2011 21:20
Mixture: CF3I_H2O_18O_asym_only.pgo
  Units               MHz
  PrintLevel          Detail
  Precision           4
  BasisOrder          boDefault
  QuantumNumberFormat J
  FitCycles           1
  FitDetails          False
  AutoReplot          True
  AllowComplex        False
  NoLineList          False
  ShowEstUnc          False
  ShowDerivatives     False
  SVDThresh     1E-15
  ScaleChanges 1
  Species: Species
    Jmax 30
    Concentration 1
    AsymmetricMolecule: AsymmetricTop
      nNuclei         1
      JAdjustSym      False
      BlockMatrix     True
      PointGroup      C2v
      Representation  Ir
      SReduction      False
      eeWt            1
      eoWt            1
      oeWt            1
      ooWt            1
      C2zAxis         a
      C2xAxis         c
      PseudoC2v       False
      FakeSym         False
      PhaseAdjust     False
      Abundance 1
      AsymmetricManifold: sym(2),K0,K1
        Initial        True
        Colour         Green
        EigenSearch    True
        LimitSearch    True
        AutoQConverge  True
        UsePopParams   False
        AsymmetricTop: sym(2),K0,K1 v=0
          Symmetry A1
          Kmin     0
          Kmax     1
          A    5600
          BBar 812.061228151106
          DJK  0.00187321832513023
          DJ   0.00013739518692128
          AsymmetricTopNucleus: sym(2),K0,K1 Nucleus1
            Spin    2.5
            AsNext False
            CHIzz -2198.87650333537
        <J,N,K|A|J,N,K> = K^2
        <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
```

```
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <sym(2),K0,K1|mu|sym(2),K0,K1>
    CartesianTransitionMoment: <sym(2),K0,K1|mu|sym(2),K0,K1> <v=0|a|v=0>
      Axis a
      Strength 1
  AsymmetricManifold: sym,K0,K1
    Initial       True
    Colour        Green
    EigenSearch   True
    LimitSearch   True
    AutoQConverge True
    UsePopParams  False
    AsymmetricTop: sym,K0,K1 v=0
      Symmetry A1
      Kmin     0
      Kmax     1
      A    5600
      BBar 811.991829422477
      DJK  0.0242106970227732
      DJ   9.25911397153272E-5
      AsymmetricTopNucleus: sym,K0,K1 Nucleus1
        Spin   2.5
        AsNext False
        CHIzz -2199.20101590993
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <sym,K0,K1|mu|sym,K0,K1>
    CartesianTransitionMoment: <sym,K0,K1|mu|sym,K0,K1> <v=0|a|v=0>
      Axis a
      Strength 1
  AsymmetricManifold: sym,K2
    Initial       True
    Colour        Green
    EigenSearch   True
    LimitSearch   True
    AutoQConverge True
    UsePopParams  False
    AsymmetricTop: sym,K2 v=0
      Symmetry A1
      Kmin     2
      Kmax     2
      A    5600
      BBar 812.037133275765
      DJK  0.0230177420339717
      DJ   0.000110566861164642
      AsymmetricTopNucleus: sym,K2 Nucleus1
        Spin   2.5
        AsNext False
        CHIzz -2198.70602173035
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K|DJK|J,N,K> = -N*(N+1)*K^2
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <sym,K2|mu|sym,K2>
    CartesianTransitionMoment: <sym,K2|mu|sym,K2> <v=0|a|v=0>
      Axis a
      Strength 1
  AsymmetricManifold: asymmetric top
    Initial       True
    Colour        Red
    EigenSearch   True
    LimitSearch   True
    AutoQConverge True
    UsePopParams  False
    AsymmetricTop: asymmetric top v=0
      Symmetry A1
      Kmin     1
      Kmax     1
      A      5600
      BBar   812.005655196239           Float
      BDelta 1.799421097283             Float
      DJ     0.000135172819363358       Float
      AsymmetricTopNucleus: asymmetric top Nucleus1
        Spin   2.5
        AsNext False
        CHIzz    -2199.25839034029           Float
        CHIxxmyy -20.4307933319512           Float
    <J,N,K|A|J,N,K> = K^2
    <J,N,K|BBar|J,N,K> = N*(N+1)-K^2
    <J,N,K-2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
    <J,N,K+2|BDelta|J,N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
    <J,N,K|DJ|J,N,K> = -N^2*(N+1)^2
  TransitionMoments: <asymmetric top|mu|asymmetric top>
    CartesianTransitionMoment: <asymmetric top|mu|asymmetric top> <v=0|a|v=0>
      Axis a
      Strength 1
```

```
Residuals before fit for AsymmetricTop for the asymmetric top manifold
  J' S' #'   J" S" #"    Observed    Calculated    Obs-Calc  StdDev
 7.5 B2  1   6.5 B1  1    8146.8610    8146.8592     0.0018 1     .00034    0 : qR1,3(4)7.5,6.5 : asymmetric top v=0  5  1  4 7.5 - asymmetric top v=0  4  1  3 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  1:<LineList>
 7.5 B1  1   6.5 B2  1    8137.9800    8137.9830    -0.0030 1     .00034    0 : qR1,4(4)7.5,6.5 : asymmetric top v=0  5  1  5 7.5 - asymmetric top v=0  4  1  4 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  2:<LineList>
 6.5 B1  2   5.5 B2  2    8123.4350    8123.4342     0.0008 1     .00028    0 : qR1,4(4)6.5,5.5 : asymmetric top v=0  5  1  5 6.5 - asymmetric top v=0  4  1  4 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  3:<LineList>
 2.5 B1  5   1.5 B2  4    8110.5000    8110.5096    -0.0096 1      .0001    0 : qR1,4(4)2.5,1.5 : asymmetric top v=0  5  1  5 2.5 - asymmetric top v=0  4  1  4 1.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  4:<LineList>
 5.5 B2  3   4.5 B1  3    8106.4500    8106.4430     0.0070 1     .00023    0 : qR1,3(4)5.5,4.5 : asymmetric top v=0  5  1  4 5.5 - asymmetric top v=0  4  1  3 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  5:<LineList>
 5.5 B1  3   4.5 B2  3    8097.4200    8097.4105     0.0095 1     .00023    0 : qR1,4(4)5.5,4.5 : asymmetric top v=0  5  1  5 5.5 - asymmetric top v=0  4  1  4 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  6:<LineList>
 4.5 B2  4   3.5 B1  4    8087.0200    8087.0124     0.0076 1     .00018    0 : qR1,3(4)4.5,3.5 : asymmetric top v=0  5  1  4 4.5 - asymmetric top v=0  4  1  3 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  7:<LineList>
 3.5 B1  5   2.5 B2  4    8079.4550    8079.4571    -0.0021 1     .00014    0 : qR1,4(4)3.5,2.5 : asymmetric top v=0  5  1  5 3.5 - asymmetric top v=0  4  1  4 2.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  8:<LineList>
 4.5 B1  4   3.5 B2  4    8077.7420    8077.7358     0.0062 1     .00018    0 : qR1,4(4)4.5,3.5 : asymmetric top v=0  5  1  5 4.5 - asymmetric top v=0  4  1  4 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  :  9:<LineList>
 4.5 B2  5   3.5 B1  5    9712.9670    9712.9697    -0.0027 1     .00015    0 : qR1,5(5)4.5,3.5 : asymmetric top v=0  6  1  6 4.5 - asymmetric top v=0  5  1  5 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 10:<LineList>
 5.5 B2  4   4.5 B1  4    9714.1070    9714.1099    -0.0029 1     .00018    0 : qR1,5(5)5.5,4.5 : asymmetric top v=0  6  1  6 5.5 - asymmetric top v=0  5  1  5 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 11:<LineList>
 4.5 B1  5   3.5 B2  5    9724.0140    9724.0127     0.0013 1     .00015    0 : qR1,4(5)4.5,3.5 : asymmetric top v=0  6  1  5 4.5 - asymmetric top v=0  5  1  4 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 12:<LineList>
 5.5 B1  4   4.5 B2  4    9725.0750    9725.0801    -0.0051 1     .00018    0 : qR1,4(5)5.5,4.5 : asymmetric top v=0  6  1  5 5.5 - asymmetric top v=0  5  1  4 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 13:<LineList>
 6.5 B2  3   5.5 B1  3    9729.3400    9729.3407    -0.0007 1     .00022    0 : qR1,5(5)6.5,5.5 : asymmetric top v=0  6  1  6 6.5 - asymmetric top v=0  5  1  5 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 14:<LineList>
 6.5 B1  3   5.5 B2  3    9740.1430    9740.1425     0.0005 1     .00022    0 : qR1,4(5)6.5,5.5 : asymmetric top v=0  6  1  5 6.5 - asymmetric top v=0  5  1  4 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 15:<LineList>
 7.5 B2  2   6.5 B1  2    9747.6130    9747.6167    -0.0037 1     .00027    0 : qR1,5(5)7.5,6.5 : asymmetric top v=0  6  1  6 7.5 - asymmetric top v=0  5  1  5 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 16:<LineList>
 3.5 B1  6   2.5 B2  5    9743.7660    9743.7827    -0.0167 1     .00012    0 : qR1,4(5)3.5,2.5 : asymmetric top v=0  6  1  5 3.5 - asymmetric top v=0  5  1  4 2.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 17:<LineList>
 7.5 B1  2   6.5 B2  2    9758.2570    9758.2572    -0.0002 1     .00027    0 : qR1,4(5)7.5,6.5 : asymmetric top v=0  6  1  5 7.5 - asymmetric top v=0  5  1  4 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 18:<LineList>
 8.5 B1  1   7.5 B2  1    9764.4780    9764.4722     0.0058 1     .00031    0 : qR1,4(5)8.5,7.5 : asymmetric top v=0  6  1  5 8.5 - asymmetric top v=0  5  1  4 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 19:<LineList>
 5.5 B1  5   4.5 B2  5   11342.7380   11342.7483    -0.0103 1     .00014    0 : qR1,6(6)5.5,4.5 : asymmetric top v=0  7  1  7 5.5 - asymmetric top v=0  6  1  6 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 20:<LineList>
 6.5 B1  4   5.5 B2  4   11344.7780   11344.7750     0.0030 1     .00016    0 : qR1,6(6)6.5,5.5 : asymmetric top v=0  7  1  7 6.5 - asymmetric top v=0  6  1  6 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 21:<LineList>
 5.5 B2  5   4.5 B1  5   11355.5050   11355.5167    -0.0117 1     .00013    0 : qR1,5(6)5.5,4.5 : asymmetric top v=0  7  1  6 5.5 - asymmetric top v=0  6  1  5 4.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 22:<LineList>
 4.5 B1  6   3.5 B2  6   11356.4350   11356.4451    -0.0101 1     .00011    0 : qR1,6(6)4.5,3.5 : asymmetric top v=0  7  1  7 4.5 - asymmetric top v=0  6  1  6 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 23:<LineList>
 7.5 B1  3   6.5 B2  3   11356.7100   11356.7108    -0.0008 1     .00019    0 : qR1,6(6)7.5,6.5 : asymmetric top v=0  7  1  7 7.5 - asymmetric top v=0  6  1  6 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 24:<LineList>
 6.5 B2  4   5.5 B1  4   11357.5060   11357.4883     0.0177 1     .00016    0 : qR1,5(6)6.5,5.5 : asymmetric top v=0  7  1  6 6.5 - asymmetric top v=0  6  1  5 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 25:<LineList>
 7.5 B2  3   6.5 B1  3   11369.3070   11369.3009     0.0061 1     .00019    0 : qR1,5(6)7.5,6.5 : asymmetric top v=0  7  1  6 7.5 - asymmetric top v=0  6  1  5 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 26:<LineList>
 4.5 B2  6   3.5 B1  6   11369.1270   11369.1382    -0.0112 1     .00011    0 : qR1,5(6)4.5,3.5 : asymmetric top v=0  7  1  6 4.5 - asymmetric top v=0  6  1  5 3.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 27:<LineList>
 8.5 B1  2   7.5 B2  2   11369.9680   11369.9700    -0.0020 1     .00022    0 : qR1,6(6)8.5,7.5 : asymmetric top v=0  7  1  7 8.5 - asymmetric top v=0  6  1  6 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 28:<LineList>
 9.5 B1  1   8.5 B2  1   11372.5270   11372.5264     0.0006 1     .00025    0 : qR1,6(6)9.5,8.5 : asymmetric top v=0  7  1  7 9.5 - asymmetric top v=0  6  1  6 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 29:<LineList>
 9.5 B2  1   8.5 B1  1   11385.0600   11385.0571     0.0029 1     .00027    0 : qR1,5(6)9.5,8.5 : asymmetric top v=0  7  1  6 9.5 - asymmetric top v=0  6  1  5 8.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 30:<LineList>
 8.5 B2  2   7.5 B1  2   11382.4620   11382.4491     0.0129 1     .00023    0 : qR1,5(6)8.5,7.5 : asymmetric top v=0  7  1  6 8.5 - asymmetric top v=0  6  1  5 7.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 31:<LineList>
 6.5 B2  5   5.5 B1  5   12970.2400   12970.2425    -0.0025 1     .00011    0 : qR1,7(7)6.5,5.5 : asymmetric top v=0  8  1  8 6.5 - asymmetric top v=0  7  1  7 5.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 32:<LineList>
 7.5 B2  4   6.5 B1  4   12972.4660   12972.4713    -0.0053 1     .00013    0 : qR1,7(7)7.5,6.5 : asymmetric top v=0  8  1  8 7.5 - asymmetric top v=0  7  1  7 6.5 : 8X_1divCF3I_someH2_18O_189439_160611 - 8X_1divCF3I_someH2_18O_189439_160611.ovr  : 33:<LineList>
```



66 Observations, 5 Parameters
Initial Average Error: 0.0105355982105031
Predicted New Error: 0.0105355982104699
Parameters:

#	Old	New	Std Dev	Change/Std	Sens	Summary	Name
1	812.005655196239	812.005655195124	.00027443	0.0000	1.35e-5	812.00566(27)	asymmetric top v=0 BBar
2	1.799421097283	1.7994210986182	.00034096	0.0000	5.42e-5	1.79942(34)	asymmetric top v=0 BDelta
3	.00013517281936358	.00013517281215483	1.7698e-6	0.0000	8.97e-8	1.352(18)e-4	asymmetric top v=0 DJ
4	-2199.25839034029	-2199.25839045116	.21474923	0.0000	.032018	-2199.26(21)	asymmetric top Nucleus1 CHIzz
5	-20.4307933319512	-20.4307847406019	.44300298	0.0000	.069928	-20.43(44)	asymmetric top Nucleus1

CHIxxmyy

Correlation Matrix

	1	2	3	4	5
1	1.000				
2	-0.026	1.000			
3	0.948	-0.017	1.000		
4	-0.334	0.040	-0.256	1.000	
5	-0.069	0.202	-0.063	-0.068	1.000