```
*Title

! KeyDebugP                ! Activate keyword debugging printouts
! TsPfDebugP                ! Activate Transition State Part. Fcn. debugging printouts
! add/elim. on singlet

   &    c4 + O3p -> p , in trans


*CalculationType

   AssociationP
   NeutralP
   ChannelsD
     2
   EJResP
   1DMasterP PCompPQ InversionPQ    !EigenvectorPQ ! EigenvaluePQ      !     !

*CalculationRanges

     TRangeP    ListDQ
            16
         ValuesL
           300    400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 2000 2500 3000

     PRangeP    ListDQ
            9
         ValuesL
            1.0e-10 1.0    10.0 100.0    300.0 500.0 760.0    3800.0    7600.0

   DZeroRangeP    ListDQ
        1
   ValuesL
      13786.35804    ! G4
!       12506.68397    !CBS-Q
!         13134.90    ! RS2/AVQZ


   ETransferRangeP

   ExpDownP NETransferDQ
      3
     ValuesL
     100.0
```

```
    400.0
    1000.0

*ConvolutionRanges

   ERangeP      StepDQ
         -5000, 100., 1500

   JRangeP    StepDQ
           1, 5, 200

*Collision

   CollMassD
    44.0      !CO2
   SigmaD
    5.0 5.0
   EpsilonD
   200. 200.


*Complex        !tM1

   NearProlateP
   NElecStatesD
        1
      ElecStatesL
         3,0.0

   NModesD
      30,1.00
   ModesL
137.7550                142.3579                188.6401
249.7285                273.3999                306.987
323.0546                349.0538                356.3079
387.7421                496.3293                544.4373
556.8174                563.7214                615.0475
620.3827                657.6757                751.7075
784.0072               1023.0496               1043.4887
1139.1843               1235.7391               1243.3857
1265.6290               1294.6423               1322.2114
1328.4415               1373.2674               1672.4867

!   FreeRotorD
```

```
!          3
!     FreeRotorL
!          2.51    3.65    2.26

     HindRotorD
          3
       HindTypeD
          1
         HindParL
          2.51    269.6    3
       HindTypeD
          1
         HindParL
          3.65    1362.3    3
       HindTypeD
          1
         HindParL
          2.26    2810.9    3

   SigRotD
      1.0

   RotConstP
      MassD
         210.98681
      RotConstD
         0.0331 0.0296 0.0237

   EVCStepD
      1.0

*Channel1

     *Fragments                    !C4

         NearProlateP
         NElecStatesD
             1
         ElecStatesL
             1 0
         NModesD
             28 1.0
         ModesL
129.9899
```

145.1465	161.7934	245.4929
252.5246	295.2872	323.8390
345.8893	434.6667	448.8016
470.9430	543.4415	560.9719
582.9054	588.7788	664.6449
745.9253	789.8109	1023.1149
1108.2264	1225.4791	1247.8006
1273.6547	1306.9353	1316.8477
1319.0484	1362.7511	2448.0946

```
!     FreeRotorD
!         2
!     FreeRotorL
!         1.92    3.01

    HindRotorD
        2
     HindTypeD
        1
       HindParL
        1.92    456.7    3
     HindTypeD
        1
       HindParL
        3.01    5499.1    3

       SigRotD
          1.

       CartesianP
       NAtomsD
          12
       PositionL
    12.0000        0.167926E-01     1.75050        0.383529E-22
    14.0031        0.347524         2.84452        0.383529E-22
    12.0000       -0.390549         0.336407       0.383529E-22
    18.9984        -1.74302         0.233055       0.383529E-22
    12.0000        0.120222        -0.344380       -1.29483
    12.0000        0.120222        -0.344380        1.29483
    18.9984         1.44181        -0.283453       -1.36303
    18.9984       -0.395737         0.287138       -2.33979
    18.9984       -0.260534         -1.61007       -1.33382
    18.9984         1.44181        -0.283453        1.36303
    18.9984       -0.260534         -1.61007        1.33382
```

18.9984 -0.395737 0.287138 2.33979

! Structure data for fragment 2, O(3P)

AtomP
NElecStatesD
3
ElecStatesL
5, 0.0
3, 158.265
1, 226.977
AtomMassD
15.99491

*TransState !tTS1

VibAdiabaticP
ElecAdiabaticP
NElecStatesD
1
ElecStatesL
3 0

RRHOP

NearProlateP

NModesD
29,1.0
ModesL

123.6524	153.4497	
171.8013	227.9747	252.7896
283.4827	301.9522	326.9301
346.6539	382.1586	453.4196
470.8662	545.8032	551.0058
581.3293	591.7135	655.0771
744.7625	788.8993	1018.7169
1093.3970	1237.6450	1244.3593
1270.1835	1306.1669	1313.6055
1317.5229	1358.7516	2205.4617

! FreeRotorD

```
!          3
!     FreeRotorL
!          1.89    2.97 2.60

     HindRotorD
          3
       HindTypeD
          1
         HindParL
          1.89      692.2    3
       HindTypeD
          1
         HindParL
          2.97      1910.0    3
       HindTypeD
          1
         HindParL
          2.60      2441.8    3

   SigRotD
        1.0

  RotConstP
  MassD
     210.98681

  RotConstD
       0.0331 0.0284 0.0221

  TSEnergyD
     1681.230489    !G4
!     3252.98935    !CBS-Q
!       2151.46        !RS2C/AVQZ

*Channel2      !

*TransState      !tTS2

     VibAdiabaticP
     ElecAdiabaticP
     NElecStatesD
          1
     ElecStatesL
          3 0
```

RRHOP

NearProlateP

NModesD
30,1.0

ModesL

38.1608	105.3802	118.3573
168.8245	239.3938	253.8768
276.6961	305.6514	308.7342
331.2045	353.2906	472.3486
517.6924	538.8183	547.0996
570.8508	628.4554	721.8470
742.4655	827.0236	1009.9360
1150.3266	1210.1186	1223.7097
1255.7336	1259.7453	1299.6215
1367.6068	1372.6182	1835.7485

```
!     FreeRotorD
!         2
!     FreeRotorL
!         1.90    2.22

    HindRotorD
        2
      HindTypeD
        1
        HindParL
        1.90      1483.3    3
      HindTypeD
        1
        HindParL
        2.22      2398.1    3
```

SigRotD
1.0

RotConstP

MassD

```
    210.98681

  RotConstD
    0.0311 0.0289 0.0221

  TSEnergyD
   -5565.439599    ! G4
!   -4549.408187 ! CBS-Q
!     -7074.19    !RS2C/AVQZ

*END
```

```
*Title

! KeyDebugP                ! Activate keyword debugging printouts
! TsPfDebugP               ! Activate Transition State Part. Fcn. debugging printouts
! add/elim. on singlet

   &   c4 + O3p -> p, in cis


*CalculationType

   AssociationP
   NeutralP
   ChannelsD
     2
   EJResP
   1DMasterP PCompPQ InversionPQ   !EigenvectorPQ ! EigenvaluePQ     !     !

*CalculationRanges

     TRangeP    ListDQ
            16
          ValuesL
            300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 2000 2500 3000

     PRangeP    ListDQ
            9
          ValuesL
            1.0e-10    1.0    10.0 100.0    300.0 500.0 760.0    3800.0    7600.0

   DZeroRangeP    ListDQ
        1
   ValuesL
     13827.20709      ! G4
!       12511.19045    !CBS-Q
!         13167.62      ! RS2/AVQZ


   ETransferRangeP

   ExpDownP NETransferDQ
      3
     ValuesL
     100.0
```

```
    400.0
    1000.0

*ConvolutionRanges

   ERangeP      StepDQ
         -5000, 100., 1500

   JRangeP    StepDQ
           1, 5, 200

*Collision

   CollMassD
    44.0      !CO2
   SigmaD
    5.0 5.0
   EpsilonD
   200. 200.


*Complex        !cM1

   NearProlateP
   NElecStatesD
        1
      ElecStatesL
         3,0.0

   NModesD
      30,1.00
   ModesL
138.2769                141.9324                180.3486
252.3281                272.9103                310.1790
320.8893                346.5242                348.5478
392.2884                512.2382                540.9362
547.1189                562.7435                620.0630
630.1910                658.4221                753.3755
784.5012                997.4967               1020.4409
1214.3002               1226.0138               1238.2795
1268.0494               1294.7973               1312.4185
1325.6842               1358.0007               1669.3930

!   FreeRotorD
```

```
!          3
!     FreeRotorL
!          2.17    3.98      2.27

     HindRotorD
          3
       HindTypeD
          1
         HindParL
          2.17    591.1    3
       HindTypeD
          1
         HindParL
          3.98    792.1    3
       HindTypeD
          1
         HindParL
          2.27    2566.0    3

   SigRotD
      1.0

   RotConstP
      MassD
         210.98681
      RotConstD
         0.03336 0.029525 0.023491

   EVCStepD
      1.0

*Channel1

     *Fragments                !C4

         NearProlateP
         NElecStatesD
             1
         ElecStatesL
             1 0
         NModesD
             28 1.0
         ModesL
129.9899
```

145.1465	161.7934	245.4929
252.5246	295.2872	323.8390
345.8893	434.6667	448.8016
470.9430	543.4415	560.9719
582.9054	588.7788	664.6449
745.9253	789.8109	1023.1149
1108.2264	1225.4791	1247.8006
1273.6547	1306.9353	1316.8477
1319.0484	1362.7511	2448.0946

```
!     FreeRotorD
!         2
!     FreeRotorL
!         1.92    3.01

    HindRotorD
        2
     HindTypeD
        1
       HindParL
        1.92    456.7    3
     HindTypeD
        1
       HindParL
        3.01    5499.1    3

       SigRotD
          1.

       CartesianP
       NAtomsD
          12
       PositionL
    12.0000        0.167926E-01     1.75050        0.383529E-22
    14.0031        0.347524         2.84452        0.383529E-22
    12.0000       -0.390549         0.336407       0.383529E-22
    18.9984        -1.74302         0.233055       0.383529E-22
    12.0000        0.120222        -0.344380       -1.29483
    12.0000        0.120222        -0.344380        1.29483
    18.9984         1.44181        -0.283453       -1.36303
    18.9984       -0.395737         0.287138       -2.33979
    18.9984       -0.260534         -1.61007       -1.33382
    18.9984         1.44181        -0.283453        1.36303
    18.9984       -0.260534         -1.61007        1.33382
```

18.9984 -0.395737 0.287138 2.33979

! Structure data for fragment 2, O(3P)

AtomP
NElecStatesD
3
ElecStatesL
5, 0.0
3, 158.265
1, 226.977
AtomMassD
15.99491

*TransState !cTS1

VibAdiabaticP
ElecAdiabaticP
NElecStatesD
1
ElecStatesL
3 0

RRHOP

NearProlateP

NModesD
31,1.0
ModesL
70.8251
77.2595 125.1889 135.4085
159.7673 229.0492 259.5427
290.8861 310.0990 324.6279
348.7087 380.3397 449.0398
482.6068 537.3371 549.1846
578.8587 591.0773 645.3215
746.2598 787.7158 1018.3334
1105.8262 1217.0650 1246.0517
1266.4679 1304.3315 1309.4141
1313.7461 1357.6879 2201.5945

```
!    FreeRotorD
!          1
!     FreeRotorL
!          2.06

     HindRotorD
          1
       HindTypeD
          1
          HindParL
           2.06      2678.1    3

   SigRotD
        1.0

  RotConstP
  MassD
     210.98681

  RotConstD
       0.032566 0.028958 0.023545

  TSEnergyD
     1929.788155    !G4
!     3626.340439    !CBS-Q
!       2395.55         !RS2C/AVQZ



*Channel2      !

*TransState      !cTS2

     VibAdiabaticP
     ElecAdiabaticP
     NElecStatesD
          1
     ElecStatesL
          3 0

   RRHOP

   NearProlateP
```

NModesD
30,1.0

ModesL

38.1608	105.3802	118.3573
168.8245	239.3938	253.8768
276.6961	305.6514	308.7342
331.2045	353.2906	472.3486
517.6924	538.8183	547.0996
570.8508	628.4554	721.8470
742.4655	827.0236	1009.9360
1150.3266	1210.1186	1223.7097
1255.7336	1259.7453	1299.6215
1367.6068	1372.6182	1835.7485

! FreeRotorD
! 3
! FreeRotorL
! 2.52 2.80 2.71

HindRotorD
3
HindTypeD
1
HindParL
2.52 935.7 3
HindTypeD
1
HindParL
2.80 1579.1 3
HindTypeD
1
HindParL
2.71 2729.6 3

SigRotD
1.0

RotConstP

MassD
210.98681

```
  RotConstD
     0.032387 0.028857 0.02231

  TSEnergyD
    -5089.238992    ! G4
!    -4027.134549    ! CBS-Q
!      -6343.44    !RS2C/AVQZ


*END
```