

(29 December 99)

## Section 3 - Input Examples

The distribution of GAMESS contains a number of short examples, named EXAM\*.INP. You should run all of these tests to be sure you have installed GAMESS correctly. The correct answers are shown in the comments preceding each of the short input tests. The "correct" answers were obtained on a RS/6000 computer, other machines may differ in the last energy digit, or the last couple of gradient digits.

The examples are listed in the rest of this section, and serve as a useful tutorial about GAMESS input.

<u>Example</u>	<u>Description</u>	<u>Page</u>
1	CH2 RHF geometry optimization	3-2
2	CH2 UHF + gradient	3-3
3	CH2 ROHF + gradient	3-4
4	CH2 GVB + gradient	3-5
5	CH2 RHF + CI gradient	3-6
6	CH2 MCSCF geometry optimization	3-7
7	HPO RHF + gradient	3-8
8	H2O RHF + MP2 gradient	3-9
9	H2O MCSCF + MCQDPT energy correction	3-10
10	H2O RHF + hessian	3-11
11	HCN RHF IRC	3-12
12	HCCH RHF geometry optimization	3-13
13	H2O RHF properties	3-14
14	H2O CI transition moment	3-16
15	C2- GVB/ROHF on 2-pi-u state	3-17
16	Si GVB/ROHF on 3-P state	3-18
17	CH2 GVB/ROHF + hessian	3-19
18	P2 RHF + hessian, effective core pot.	3-20
19	NH spin-orbit coupling	3-21
20	I- exponent TRUDGE optimization	3-22
21	CH3 OS-TCSCF hessian	3-23
22	H3CN UHF + UMP2 energy	3-25
23	SiH3- PM3 geometry optimization	3-26
24	H2O SCRF test case	3-27
25	? internal coordinate example	3-28
26	H3PO localized orbital test	3-31
27	NH3 DRC example	3-32
28	H2O-NH3 Morokuma decomposition	3-33
29	FNH2OH surface scan	3-34
30	HCONH2(H2O)3 effective fragment solvation	3-35
31	H2O PCM test case	3-36

```
! EXAM01.
!   1-A-1 CH2   RHF geometry optimization using GAMESS.
!
!   Although internal coordinates are used (COORD=ZMAT),
!   the optimization is done in Cartesian space (NZVAR=0).
!   This run uses a criterion (OPTTOL) on the gradient
!   which is tighter than is normally used.
!
!   This job tests the sp integral module, the RHF module,
!   and the geometry optimization module.
!
!   Using the default search METHOD=STANDARD,,
!   FINAL E= -37.2322678015, 8 iters, RMS grad= .0264308
!   FINAL E= -37.2308175316, 7 iters, RMS grad= .0320881
!   FINAL E= -37.2375723414, 7 iters, RMS grad= .0056557
!   FINAL E= -37.2379944431, 6 iters, RMS grad= .0017901
!   FINAL E= -37.2380387832, 8 iters, RMS grad= .0003391
!   FINAL E= -37.2380397692, 6 iters, RMS grad= .0000030
!
!$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE COORD=ZMT NZVAR=0 $END
!$SYSTEM TIMLIM=2 MEMORY=100000 $END
!$STATPT OPTTOL=1.0E-5 $END
!$BASIS  GBASIS=STO NGAUSS=2 $END
!$GUESS  GUESS=HUCKEL $END
!$DATA
Methylene...1-A-1 state...RHF/STO-2G
Cnv  2

C
H  1 rCH
H  1 rCH  2 aHCH

rCH=1.09
aHCH=110.0
$END
```

```

! EXAM02.
!   3-B-1 CH2   UHF calculation on methylene ground state.
!
!   This test uses the default choice, COORD=UNIQUE, to
!   enter the molecule.  Only the symmetry unique atoms
!   are given, and they must be given in the orientation
!   which GAMESS expects.
!
!   This job tests the UHF energy and the UHF gradient.
!   In addition, the orbitals are localized.
!
!   The initial energy is -37.228465066.
!   The FINAL energy is -37.2810867258 after 11 iterations.
!   The unrestricted wavefunction has <S**2> = 2.013.
!   Mulliken, Lowdin charges on C are -0.020584, 0.018720.
!   The spin density at Hydrogen is -0.0167104.
!   The dipole moment is 0.016188.
!   The RMS gradient is 0.027589766.
!   FINAL localization sums are 30.57 and 25.14 Debye**2.
!
$CONTRL SCFTYP=UHF MULT=3 RUNTYP=GRADIENT LOCAL=BOYS $END
$SYSTEM TIMLIM=1 MEMORY=100000 $END
$BASIS  GBASIS=STO NGAUSS=2 $END
$GUESS  GUESS=HUCKEL $END
$DATA
Methylene...3-B-1 state...UHF/STO-2G
Cnv  2

Carbon      6.0
Hydrogen    1.0    0.0    0.82884    0.7079
$END

```

```
! EXAM03.
!   3-B-1 CH2 ROHF calculation on methylene ground state.
!   The wavefunction is a pure triplet state (<S**2> = 2),
!   and so has a higher energy than the second example.
!
!   For COORD=CART, all atoms must be given, and as in the
!   present case, these may be in an unoriented geometry.
!   GAMESS deduces which atoms are unique, and orients
!   the molecule appropriately. The geometry here is thus
!   identical to the second example.
!
!   This job tests the ROHF wavefunction and gradient code.
!   It also tests the direct SCF procedure.
!
!   The initial energy is -37.228465066.
!   The FINAL energy is -37.2778767089 after 7 iterations.
!   Mulliken, Lowdin charges on C are -0.020346, 0.019470.
!   The Hydrogen atom spin density is 0.0129735.
!   The dipole moment is 0.025099 Debye.
!   The RMS gradient is 0.027505548
!
$CONTRL SCFTYP=ROHF MULT=3 RUNTYP=GRADIENT COORD=CART $END
$SYSTEM TIMLIM=1 MEMORY=100000 $END
$SCF DIRSCF=.TRUE. $END
$BASIS GBASIS=STO NGAUSS=2 $END
$GUESS GUESS=HUCKEL $END
$DATA
Methylene...3-B-1 state...ROHF/STO-2G
Cnv 2

Hydrogen 1.0 0.82884 0.7079 0.0
Carbon 6.0
Hydrogen 1.0 -0.82884 0.7079 0.0
$END
```

```

! EXAM04.
!   1-A-1 CH2   TCSCF calculation on methylene.
!   The wavefunction has two configurations, exciting
!   the carbon sigma lone pair into the out of plane p.
!
!   Note that the Z-matrix used to input the molecule
!   can include identifying integers after the element
!   symbol, and that the connectivity can then be given
!   using these labels rather than integers.
!
!   This job tests the GVB wavefunction and gradient.
!
!   The initial GVB-PP(1) energy is -37.187342653.
!   The FINAL energy is -37.2562020559 after 10 iters.
!   The GVB CI coefs are 0.977505 and -0.210911, giving
!   a pair overlap of 0.64506.
!   Mulliken, Lowdin charges for C are 0.020810, 0.055203.
!   The dipole moment is 1.249835.
!   The RMS gradient = 0.019618475.
!
$CONTRL SCFTYP=GVB  RUNTYP=GRADIENT  COORD=ZMT  $END
$SYSTEM TIMLIM=1  MEMORY=100000  $END
$BASIS  GBASIS=STO  NGAUSS=2  $END
$SCF    NCO=3  NSETO=0  NPAIR=1  $END
$DATA
Methylene...1-A-1 state...GVB...one geminal pair...STO-2G
Cnv  2

C1
H1  C1 rCH
H2  C1 rCH  H1 aHCH

rCH=1.09
aHCH=99.0
$END
! normally a GVB-PP calculation will use GUESS=MOREAD
$GUESS  GUESS=HUCKEL  $END

```

```

! EXAM05
!   CH2   CI calculation.
!   The wavefunction is RHF + CI-SD, within the minimal
!   basis, containing 55 configurations. Two CI roots
!   are found, and the gradient of the higher state is
!   then computed.
!
!   Note that CI gradients have several restrictions,
!   which are further described in the $LAGRAN group.
!
!   FINAL energy of RHF = -38.3704885128 after 10 iters.
!   State 1 EIGENvalue = -38.4270674136, c(1) = 0.970224
!   State 2 EIGENvalue = -38.3130036824, c(29) = 0.990865
!   The upper state dipole moment is 0.708275 Debye.
!   The upper state has RMS gradient 0.032264079
!
$CONTRL SCFTYP=RHF CITYP=GUGA RUNTYP=GRADIENT $END
$SYSTEM TIMLIM=3 MEMORY=300000 $END
$BASIS  GBASIS=STO NGAUSS=3 $END
$GUESS  GUESS=HUCKEL $END
!   look at all state symmetries, by using C1 symmetry
$CIDRT  GROUP=C1 IEXCIT=2 NFZC=1 NDOC=3 NVAL=3 $END
!   ground state is 1-A-1, 1st excited state is 1-B-1
$GUGDIA NSTATE=2 $END
!   compute properties of the 1-B-1 state
$GUGDM  NFLGDM(1)=1,1 IROOT=2 $END
!   compute gradient of the 1-B-1 state
$GUGDM2 WSTATE(1)=0.0,1.0 $END
$DATA
Methylene...CI...STO-3G basis
Cnv    2

Carbon    6.0
Hydrogen  1.0      0.0      0.82884      0.7079
$END

```

```

! EXAM06.
!   1-A-1 CH2   MCSCF methylene geometry optimization.
!   The two configuration ansatz is the same as used in
!   the fourth example.
!
!   The optimization is done in internal coordinates,
!   as NZVAR is non-zero.  Since a explicit $ZMAT is
!   given, these are used for the internal coordinates,
!   rather than those used to enter the molecule in
!   the $DATA.  (Careful examination of this trivial
!   triatomic's input shows that $ZMAT is equivalent
!   to $DATA in this case.  You would normally give
!   $ZMAT only if it is somehow different.)
!
!   This job tests the MCSCF wavefunction and gradient.
!
!   At the initial geometry:
!   The initial energy is -37.187342653,
!   the FINAL E= -37.2562020559 after 14 iterations,
!   the RMS gradient is 0.0256396.
!
!   After 4 steps,
!   FINAL E= -37.2581791686, RMS gradient=0.0000013,
!   r(CH)=1.1243359, ang(HCH)=98.8171674
!
$CONTRL SCFTYP=MCSCF RUNTYP=OPTIMIZE NZVAR=3 COORD=ZMT $END
$SYSTEM TIMLIM=5 MEMORY=300000 $END
$BASIS  GBASIS=STO NGAUSS=2 $END
$DATA
Methylene...1-A-1 state...MCSCF/STO-2G
Cnv  2

C
H 1 rCH
H 1 rCH 2 aHOH

rCH=1.09
aHOH=99.0
$END
$ZMAT  IZMAT(1)=1,1,2,   1,1,3,   2,2,1,3  $END
!
! Normally one starts a MCSCF run with converged SCF
! orbitals, as Huckel orbitals normally do not converge.
! Even if they do converge, the extra iterations are
! very expensive, so use MOREAD for your runs!
!
$GUESS  GUESS=HUCKEL $END
!
! two active electrons in two active orbitals.
! must find at least two roots since ground state is 3-B-1
!
$DET    NCORE=3 NACT=2 NELS=2 NSTATE=2 $END

```

```
! EXAM07.
! 1-A' HPO RHF calculation using GAMESS.
! This job tests the HONDO integral and gradient package,
! due to the d function on phosphorus. The input also
! illustrates the use of a more flexible basis set than
! the methylene examples.
! Although HUCKEL would be better, HCORE is tested.
!
! The initial energy is -397.591192627,
! the FINAL E= -414.0945320854 after 18 iterations,
! The dipole moment is 2.535169.
! The RMS gradient is 0.023723942.
!
$CONTRL SCFTYP=RHF RUNTYP=GRADIENT $END
$SYSTEM TIMLIM=20 MEMORY=300000 $END
$GUESS GUESS=HCORE $END
$DATA
HP=O ... 3-21G+* RHF calculation at STO-2G* geometry
Cs

Phosphorus 15.0
  N21 3
  L 1
  1 0.039 1.0 1.0
  D 1
  1 0.55 1.0

Oxygen 8.0 1.439
  N21 3

Hydrogen 1.0 -0.3527854 1.36412
  N21 3

$END
```



```
! EXAM08.
! 1-A-1 H2O RHF + MP2 gradient calculation.
! This job generates RHF orbitals which should be saved
! for use with EXAM9. This run, together with EXAM9,
! shows a much more typical MCSCF calculation, which
! should always be started with some sort of SCF MOs.
! This job also tests the 2nd order Moller-Plesset code.
!
! The FINAL E is -75.5854099058 after 10 iterations.
! E(MP2) is -75.7060361996, RMS grad=0.017449524
! dipole moments are SCF=2.435689, MP2=2.329368
!
$CONTRL SCFTYP=RHF MPLEVL=2 RUNTYP=GRADIENT $END
$SYSTEM TIMLIM=2 MEMORY=100000 memddi=1 parall=.true. $END
$BASIS GBASIS=N21 NGAUSS=3 $END
$GUESS GUESS=HUCKEL $END
$DATA
Water...RHF/3-21G...exp.geom...R(OH)=0.95781,A(HOH)=104.4776
Cnv      2

OXYGEN      8.0
HYDROGEN    1.0    0.0    0.7572157    0.5865358
$END
```

```

! EXAM09.
!   1-A-1 H2O    2nd order MC-QDPT calculation
!   This job finds the Full Optimized Reaction Space
!   MCSCF (or CAS-SCF) wavefunction for water.  Its
!   initial RHF orbitals are taken from EXAM8.
!   The MCSCF wavefunction contains 225 determinants,
!   which includes 105 singlet configurations.
!   The second order perturbation theory correction
!   to the MCSCF energy is then obtained, using the
!   slower code that produces information about
!   what weight percent the MCSCF comprises in the
!   first order wavefunction.
!
!   MCSCF:
!   On the 1st iteration, the energy is -75.601726235.
!   The FINAL E= -75.6386218833 after 13 iterations,
!   with c(1) = 0.988446 and dipole moment = 2.301626
!
!   MC-QDPT:
!   E(MCSCF)= -75.6386218833, E(MP2)= -75.7109706204
!   the 2nd order correction has 2 terms, semi-internal
!   is -0.03446957 and external -0.03787916 Hartree,
!   and the MCSCF reference weight is 98.4%.
!
$CONTRL SCFTYP=MCSCF MLEVEL=2 $END
$SYSTEM TIMLIM=8 MEMORY=300000 $END
$BASIS  GBASIS=N21 NGAUSS=3 $END
---- EXPERIMENTAL GEOM, R(OH)=0.95781A, HOH=104.4776 DEG.
$DATA
WATER...3-21G BASIS...FORS-MCSCF...EXPERIMENTAL GEOMETRY
Cnv 2

Oxygen      8.0
Hydrogen    1.0   0.0   0.7572157   0.5865358
$END
$GUESS  GUESS=MOREAD  NORB=13 $END
$DET    NCORE=1 NACT=6 NELS=8 $END
$MCQDPT NSTATE=1 ISTSYM=1 INORB=0 REFWGT=.TRUE. $END
---- CONVERGED 3-21G WATER VECTORS, E=-75.585409913 - - -
$VEC
  1  1  0.98323195E+00  0.95883436E-01  0.00000000E+00 ...
... vectors deleted to save paper ...
 13  3  0.35961579E+00  0.28728587E+00  0.35961579E+00
$END

```

```

! EXAM 10.
!   This run duplicates the first column of table 6 in
!   Y.Yamaguchi, M.Frisch, J.Gaw, H.F.Schaefer, and
!   J.S.Binkley  J.Chem. Phys. 1986, 84, 2262-2278.
!
!   FINAL energy at the VIB 0 geometry is -74.9659012159.
!
!   If run with METHOD=ANALYTIC,
!   the FREQUencies are 2170.05, 4140.00, and 4391.07
!   the INTENSities are 0.17129, 1.04807, and 0.70930
!   the mean POLARIZABILITY is 0.40079
!
!   If run with METHOD=NUMERIC, NVIB=2,
!   the FREQUencies are 2170.14, 4140.18, and 4391.12
!   the INTENSities are 0.17169, 1.04703, and 0.70909
!
$CONTRL SCFTYP=RHF RUNTYP=HESSIAN UNITS=BOHR NZVAR=3 $END
$SYSTEM TIMLIM=4 MEMORY=100000 $END
$FORCE  METHOD=ANALYTIC  $END
$CPHF   POLAR=.TRUE. $END
$BASIS  GBASIS=STO NGAUSS=3 $END
$DATA
Water at the RHF/STO-3G equilibrium geometry
CNV      2

OXYGEN      8.    0.0    0.0                0.0702816679
HYDROGEN    1.    0.0    1.4325665478   -1.1312080153
$END
$ZMAT      IZMAT(1)=1,1,2,    1,1,3,    2,2,1,3  $END
$GUESS     GUESS=HUCKEL  $END

```

```

! EXAM 11.
! 1A' HCN          RHF Intrinsic Reaction Coordinate
! This job tests the reaction path finder.  The reaction
! IS Followed back to the HNC isomer.  Four points on the
! IRC (counting the saddle point) are found,
! Pt.   R(N-C)   R(N-H)   A(HNC)   Energy   distance
! T.S.  1.22136  1.43764  52.993   -91.5648510  0.0
! 1     1.22533  1.33296  58.476   -91.5673097  0.29994
! 2     1.22802  1.23827  64.747   -91.5735346  0.59986
! 3     1.22974  1.16350  72.039   -91.5814775  0.89968
!
$CONTRL SCFTYP=RHF RUNTYP=IRC NZVAR=3 $END
$SYSTEM TIMLIM=5 MEMORY=400000 $END
$IRC     PACE=GS2 SADDLE=.TRUE. TSENGY=.TRUE.
        FORWRD=.FALSE. NPOINT=3 $END
$GUESS  GUESS=HUCKEL $END
$ZMAT   IZMAT(1)=1,1,2 1,1,3 2,2,1,3 $END
$BASIS  GBASIS=STO NGAUSS=3 $END
$DATA
HYDROGEN CYANIDE...STO-3G...INTRINSIC REACTION COORDINATE
CS
NITROGEN   7.0   -.0004620071   .0002821165   .0000000000
CARBON     6.0   1.2208931990  -.0003427488   .0000000000
HYDROGEN   1.0   .8654562191   1.1478852258   .0000000000
$END
$HESS
ENERGY IS      -91.5648510307 E(NUC) IS      23.4154954113
1 1 1.10665682E+00 1.58946320E-02 0.00000000E+00...
... 2nd derivatives deleted to save paper ...
9 2-8.04548379E-09 0.00000000E+00 0.00000000E+00-1.42096449E-08
$END

```

```
! EXAM 12.
!   This job illustrates linear bends, for acetylene.
!   The optimal RHF/STO-2G geometry is located.
!
!   At the input geometry,
!   the FINAL E= -73.5036974734 after 7 iterations,
!   and the RMS gradient is 0.1506891.
!
!   At the final geometry, 7 steps later,
!   the FINAL E= -73.6046483165, RMS gradient=0.0000028,
!   R(CC)=1.1777007 and R(CH)=1.0749435.
!
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE NZVAR=5 $END
$SYSTEM TIMLIM=6 MEMORY=100000 $END
$BASIS  GBASIS=STO NGAUSS=2 $END
$GUESS  GUESS=HUCKEL $END
$DATA
Acetylene geometry optimization in internal coordinates
Dnh      4

CARBON      6.0    0.0    0.0    0.70
HYDROGEN    1.0    0.0    0.0    1.78
$END
$ZMAT  IZMAT(1)=1,1,2,    1,1,3,    1,2,4,
          5,1,2,4,    5,2,1,3 $END
----- XZ is 1st plane for both bends -----
$LIBE  APTS(1)=1.0,0.0,0.0,1.0,0.0,0.0 $END
```

```

! EXAM 13.
! This run duplicates the POLYATOM calculation of
! D.Neumann + J.W.Moskowitz, J.Chem.Phys. 49,2056(1968)
! SCF convergence is a bit better today, so some of the
! results are not precisely the same.
!
! V(NE) = -199.1343264099
! V(EE) = 37.8955167210 T = 75.9557584991
! V(NN) = 9.2390200836 E(TOT)= -76.0440311061
! Mulliken charge(O)=-0.647397 Bond Order=0.905
! Density: O=286.491824 H=0.404989
! Moments: DZ= 2.093290
! QXX=-2.388658 QYY= 2.495388 QZZ=-0.106730
! OXXZ=-0.890362 OYYZ= 2.186853 OZZZ=-1.296490
! Electric field/gradient: H(YZ)=+/-0.365168
! O(Z)=-0.060033 H(Y)=+/-0.006572 H(Z)=0.001233
! O(XX)=1.904867 O(YY)=-1.735891 O(ZZ)=-0.168977
! H(XX)=0.301208 H(YY)=-0.258153 H(ZZ)=-0.043055
! Potential: V(O)=-22.330374 V(H)=-1.006648
!
$CONTRL SCFTYP=RHF RUNTYP=ENERGY UNITS=BOHR ISPHER=1 $END
$SYSTEM TIMLIM=15 MEMORY=300000 $END
$GUESS GUESS=HUCKEL $END
$ELMOM IEMOM=3 $END
$ELFLDG IEFLD=2 $END
$ELPOT IEPOT=1 $END
$ELDENS IEDEN=1 $END
$DATA
Water...properties test...(10,5,2/4,1)/[5,3,2/2,1] basis
Cnv 2

Oxygen 8.0
S 2
  1 31.3166 0.243991
  2 76.232 0.152763
S 3
  1 290.785 0.904785
  2 1424.0643 0.121603
  3 4643.4485 0.029225
S 2
  1 4.6037 0.264438
  2 12.8607 0.458240
S 2
  1 0.9311 1.051534
  2 9.7044 -0.140314
S 1
  1 0.2825 1.0
P 3
  1 7.90403 0.124190
  2 35.1832 0.019580
  3 2.30512 0.394730
P 1
  1 0.21373 1.0
P 1
  1 0.71706 1.0
D 1
  1 1.5 1.0
D 1

```

1	0.5		1.0	
Hydrogen	1.0	0.0	1.428036	1.0957706
S	3			
1	0.65341		0.817238	
2	2.89915		0.231208	
3	19.2406		0.032828	
S	1			
1	0.17758		1.0	
P	1			
1	1.0		1.0	

\$END

```

! EXAM 14.
! CI transition moments. Water, using RHF/STO-3G MOs.
! All orbitals are occupied, transition is 1-1A1 to 2-1A1.
!
! E(STATE 1)= -75.0101113548, E(STATE 2)= -74.3945819375
! Dipole LENGTH is <Q>=0.392614
! Dipole VELOCITY is <d/dQ>=0.368205
!
$CONTRL SCFTYP=NONE CITYP=GUGA RUNTYP=TRANSITN UNITS=BOHR $END
$SYSTEM TIMLIM=1 MEMORY=100000 $END
$BASIS GBASIS=STO NGAUSS=3 $END
!           standard SD-CI calculation
$DRT1  GROUP=C2V IEXCIT=2 NFZC=1 NDOC=4 NVAL=2 $END
$TRANST NFZC=1 IROOTS(1)=1,2 $END
$DATA
WATER MOLECULE...STO-3G...TRANSITION MOMENT
CNV      2

OXYGEN      8.0   0.0   0.0   0.0
HYDROGEN    1.0   0.0   1.428  -1.096
$END
!           standard SD-CI calculation
$CIDRT1 GROUP=C2V IEXCIT=2 NFZC=1 NDOC=4 NVAL=2 $END

--- RHF ORBITALS --- GENERATED AT 09:24:04    18-FEB-88
WATER MOLECULE...STO-3G...TRANSITION MOMENT
E(RHF)= -74.9620539825, E(NUC)=  9.2384802989,    8 ITERS
$VEC1
 1  1  9.94117078E-01  2.66680164E-02  0.00000000E+00 ...
... vectors deleted to save paper ...
 7  2 -8.42653177E-01  8.42653177E-01
$END

```



```
! EXAM 15.
!   C2- diatom, in the electronic state doublet-pi-u.
!   This illustrates a open shell SCF calculation, using
!   fed in coupling coefficients, and the GVB/ROHF code.
!
!   The FINAL energy is -75.5579181071 after 8 iterations.
!
$CONTRL SCFTYP=GVB MULT=2 ICHARG=-1 UNITS=BOHR $END
$SYSTEM TIMLIM=15 MEMORY=300000 $END
$BASIS  GBASIS=DH NDFUNC=1 POLAR=DUNNING $END
$DATA
C2-...DOUBLET-PI-UNGERADE...OPEN SHELL SCF
DNH      4

CARBON      6.0      0.0  0.0  -1.233
$END
$GUESS  GUESS=MOREAD NORB=30
        NORDER=1 IORDER(5)=7,5,6 $END
$SCF    NCO=5 NSETO=1 NO=2 COUPLE=.TRUE.
        F(1)=1.0, 0.75
        ALPHA(1)=2.0, 1.5, 1.00
        BETA(1)=-1., -.75, -0.5 $END

--- RHF ORBITALS --- GENERATED AT 14:05:16THU MAR 24/88
CC R(C-C) = 2 * 1.233 BOHR BAS=831+1D
E(RHF)= -75.3856001855, E(NUC)= 14.5985401460, 18 ITERS
$VEC
1 1-7.06500288E-01-1.39103044E-03-3.57452331E-04 ...
... vectors deleted to save paper ...
$END
```

```
! EXAM 16.
! ROHF/GVB on Si 3-P state, using Gordon's 6-31G basis.
!
! The purpose of this example is two-fold, namely to
! show off the open shell capabilities of the GVB code,
! and to emphasize that the 6-31G basis for Si in GAMESS
! is Mark Gordon's version. The basis stored in GAMESS is
! completely optimized, whereas Pople's uses the core from
! from a 6-21G set, reoptimizing only the -31G part.
! The energy from Pople's basis would be only -288.828405.
!
! Jacobi diagonalization is intrinsically slow, but in this
! case results in pure subspecies in degenerate p irreps.
! In fact, these may be labeled in the highest Abelian
! subgroup of the atomic point group Kh.
!
! The FINAL energy is -288.8285729745 after 7 iterations.
!
$CONTRL SCFTYP=GVB MULT=3 $END
$SYSTEM TIMLIM=2 MEMORY=100000 KDIAG=3 $END
$BASIS GBASIS=N31 NGAUSS=6 $END
$DATA
Si...3-P term...ROHF in full Kh symmetry
Dnh 2

Silicon      14.
$END
$GUESS GUESS=HUCKEL $END
$SCF NCO=6 NSETO=1 NO=3 COUPLE=.TRUE.
      F(1)=1.0, 0.3333333333333333
      ALPHA(1)=2.0, 0.666666666666667, 0.166666666666667
      BETA(1)=-1.0, -0.333333333333333, -0.166666666666667
$END
```

```
! EXAM 17.
! Analytic hessian for an open shell SCF function.
! Methylene's 1-B-1 excited state.
! FINAL energy= -38.3334724780 after 8 iterations.
! The FREQUencies are 1224.19, 3563.44, 3896.23
! The INTENSities are 0.13317, 0.21652, 0.14589
! The mean POLARIZABILITY is 0.53018
!
$CONTRL SCFTYP=GVB MULT=1 RUNTYP=HESSIAN UNITS=BOHR $END
$SYSTEM TIMLIM=4 MEMORY=100000 $END
$CPHF POLAR=.TRUE. $END
$BASIS GBASIS=STO NGAUSS=3 $END
$SCF NCO=3 NSETO=2 NO(1)=1,1 NPAIR=0 $END
$ZMAT IZMAT(1)=1,1,2, 1,1,3, 2,2,1,3 $END
$GUESS GUESS=HUCKEL $END
$DATA
METHYLENE...1-B-1 STATE...ROHF...STO-3G BASIS
CNV 2

CARBON 6.0 0.0 0.0 0.0041647278
HYDROGEN 1.0 0.0 1.8913952563 0.7563907037
$END
```

```
! EXAM 18.
! effective core potential...diatomic P2...RHF/CEP-31G*
! See Stevens,Basch,Krauss, J.Chem.Phys. 81,6026-33(1984).
! GAMESS FINAL E= -12.6956518702, FREQ=913.17
! A separate run gives E(P)= -6.32635, so De= 26.95 kcal/mol
!
$CONTRL SCFTYP=RHF RUNTYP=HESSIAN ECP=SBKJC NZVAR=1 $END
$SYSTEM TIMLIM=15 MEMORY=900000 $END
$GUESS GUESS=HUCKEL $END
$ZMAT IZMAT(1)=1,1,2 $END
$DATA
diatomic phosphorous
Dnh 4

PHOSPHORUS 15.0 0.0000000000 0.0000000000 0.9393077548
  SBKJC
  D 1
    1 0.45 1.0

$END
```

```

! EXAM 19.
! Spin-orbit coupling example.
! This run duplicates the results shown in Table 3 of
! T.R.Furlani, H.F.King, J.Chem.Phys. 82, 5577-83(1985),
! GAMESS 1e-= 114.3851, 2e-= -49.4168, lit=114.38,-49.42
!
! Energies for the singlet CI are
!   State=  1 Energy =  -54.868531216 (1-delta)
!   State=  2 Energy =  -54.868531216 (1-delta)
!   State=  3 Energy =  -54.798836731 (1-sigma-plus)
! Energies for the triplet CI are
!   State=  1 Energy =  -54.938225701 (3-sigma-minus)
! Final energies of all 6 levels in the pi**2 configuration,
! after diagonalization of the spin-orbit Hamiltonian, are
! BREIT RELATIVE E= -15296.570, -15296.432, -15296.432,
! BREIT RELATIVE E= 0.0, 0.0, and +15296.570 wavenumbers.
! If run as OPERAT=HSO1, with ZEFF taken as true atomic Z,
! then inclusion of only the 1e- operator is 114.3851, and
! ZEFF RELATIVE E= -15296.859, -15296.432, -15296.432,
! ZEFF RELATIVE E= 0.0, 0.0, and +15296.859 wavenumbers.
!
! Why are there six levels? The singlet-delta is two roots,
! the singlet-sigma-plus is a third. During the CI, the
! spatial triplet-sigma-minus is one CSF, with alpha/alpha
! spin, hence IROOTS=3,1. The final spin-orbit Hamiltonian
! includes all three triplet spin states, namely adding the
! ab+ba and beta/beta triplets. So, 2+1+3=6 levels. You
! can work out for yourself these have the quantum number
! omega=0,0,1,2. Only the omega=0 states can interact,
! raising the triplet's degeneracy and slightly affecting
! the singlet-sigma-plus state's position.
!
! Note that the lower multiplicity DRT1 is done in C1
! symmetry to generate both components of the delta state.
!
$CONTRL SCFTYP=NONE MULT=3 CITYP=GUGA RUNTYP=TRANSITN
        UNITS=BOHR $END
$SYSTEM TIMLIM=2 MEMORY=900000 $END
$BASIS  GBASIS=N31 NGAUSS=6 $END
$TRANST OPERAT=HSO2 NFZC=3 NOCC=5 NUMVEC=1 NUMCI=2
        IROOTS(1)=3,1 $END
$DRT1   GROUP=C1  IEXCIT=2 NFZC=3 NDOC=1 NVAL=1 $END
$DRT2   GROUP=C4V IEXCIT=2 NFZC=3 NALP=2 $END
$DATA
Imidogen radical
Cnv 4

Nitrogen      7.0
Hydrogen      1.0      0.0      0.0      1.9748
$END
--- ROHF ORBITALS --- GENERATED AT 12:04:18 29 MAR 90 ( 88)
IMIDOGEN RADICAL
E(ROHF)= -54.9382257007, E(NUC)=      3.5446627507,      8 ITERS
$VEC1
...orbitals omitted to save space...
$END

```

```
!EXAM 20.
! Optimize an orbital exponent.
! The SBKJC basis for I consists of 5 gaussians, in a -41
! type split. The exponent of a diffuse L shell for
! iodide ion is optimized (6th exponent overall). The
! optimal exponent turns out to be 0.036713, with a
! corresponding FINAL energy of -11.3010023066
!
$CONTRL SCFTYP=RHF RUNTYP=TRUDGE ICHARG=-1 ECP=SBKJC $END
$SYSTEM TIMLIM=30 MEMORY=300000 $END
$TRUDGE OPTMIZ=BASIS NPAR=1 IEX(1)=6 $end
$GUESS GUESS=HUCKEL $END
$DATA
I- ion
Dnh 2

Iodine 53.0
  SBKJC
  L 1
    1 0.02 1.0

$END
```

```

! EXAM 21.
!   Open shell two configuration SCF analytic hessian.
!       M.Duran, Y.Yamaguchi, H.F.Schaefer III
!       J.Phys.Chem. 1988, 92, 3070-3075.
!   Least motion insertion of CH into H2, which leads to
!   a 3rd order hypersaddle point on the 2-B-1 surface.
!   Literature values are
!       FINAL E=-39.25104,      C1=0.801,      C2=-0.598
!       FREQ= 4805i, 1793i, 1317i, 989, 2914, 3216
!       mean POLARIZABILITY=2.05
!   GAMESS obtains
!       FINAL E=-39.2510351249, C1=0.801141, C2=-0.598476
!       FREQ= 4805.53i, 1793.00i, 1317.43i,
!       FREQ= 988.81, 2913.52, 3216.42
!       INTENS= 4.54563, 0.09731, 0.00768
!       mean POLARIZABILITY=2.04655
$CONTRL SCFTYP=GVB MULT=2 RUNTYP=HESSIAN $END
$SYSTEM TIMLIM=25 MEMORY=100000 $END
$CPHF POLAR=.TRUE. $END
$GUESS GUESS=MOREAD NORB=16 NORDER=1 IORDER(4)=6,4,5 $END
$SCF NCO=3 NSETO=1 NO=1 NPAIR=1 CICOEF(1)=0.7,-0.7 $END
$DATA
Insertion of CH into H2...OS-TCSCF ansatz...DZ basis
CNV 2

CARBON  6.0  0.0000000000  0.0000000000  -0.0001357549
S  6
  1  4232.61  0.002029
  2  634.882  0.015535
  3  146.097  0.075411
  4  42.4974  0.257121
  5  14.1892  0.596555
  6  1.9666  0.242517
S  1
  1  5.1477  1.0
S  1
  1  0.4962  1.0
S  1
  1  0.1533  1.0
P  4
  1  18.1557  0.018534
  2  3.9864  0.115442
  3  1.1429  0.386206
  4  0.3594  0.640089
P  1
  1  0.1146  1.0

HYDROGEN  1.0  0.0000000000  0.0000000000  1.0922959062
DH  0  1.2  1.2

HYDROGEN  1.0  0.0000000000  0.4152229538  -1.4824967459
DH  0  1.2  1.2

$END
--- these are 2-A1 ROHF vectors ---
--- ROHF ORBITALS --- GENERATED AT 08:23:42 27 JUN 90 (178)
INSERTION OF CH INTO H2...OS-TCSCF ANSATZ...DZ BASIS
E(ROHF)= -39.2316245004, E(NUC)= 8.0760320442, 12 ITERS

```

```
$VEC  
1 1 6.01223299E-01 4.37813104E-01 ...  
... vectors deleted to save paper ...  
16 4-2.12429766E-02  
$END
```



```
! EXAM22.
!
!   3-A-2 H3CN   UMP2/6-31G**//UHF/6-31G*
!
!   The FINAL UHF energy= -94.0039683676 after 13 iters.
!   The E(MP2) energy= -94.2315757758
!
$CONTRL SCFTYP=UHF MULT=3 RUNTYP=ENERGY MLEVEL=2
        COORD=ZMT $END
$SYSTEM TIMLIM=30 MEMORY=300000 $END
$BASIS  GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=0 $END
$GUESS  GUESS=HUCKEL $END
$DATA
Methylnitrene...UHF/6-31G* structure
Cnv 3

N
C  1  rCN
H  2  rCH  1  aHCN
H  2  rCH  1  aHCN  3  120.0
H  2  rCH  1  aHCN  3 -120.0

rCN=1.4329216
rCH=1.0876477
aHCN=110.21928
$END
```

```

! EXAM23.
!   semiempirical calculation, using the MOPAC/GAMESS combo
!   AM1 gets the geometry disasterously wrong!
!
!   initial geometry,           MNDO           AM1           PM3
!   FINAL HEAT OF FORMATION     105.14088    93.45997    46.89387
!   RMS gradient                 0.0818157    0.1008587    0.0366232
!   final geometry (# steps),    8            11           10
!   FINAL HEAT OF FORMATION     46.45649    -1.81716    -2.79647
!   RMS gradient                 0.0000246    0.0000294    0.0000015
!   r(SiH)                      1.42117     1.45813     1.52104
!   a(HSiH)                     101.962     120.000     96.280
!
!   At the final PM3 geometry, the charge on Silicon is -.4681,
!   and the dipole moment is 2.345322 Debye.
!
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE COORD=ZMT ICHARG=-1 $END
$SYSTEM TIMLIM=5 MEMORY=200000 $END
$BASIS  GBASIS=PM3 $END
$DATA
Silyl anion...comparison of semiempirical models
Cnv 3

Si
H 1  rSiH
H 1  rSiH  2  aHSiH
H 1  rSiH  2  aHSiH  3  aHSiH  -1

rSiH=1.15
aHSiH=110.0
$END

```

```
! EXAM24.
! Self-consistent reaction field test, of water in water.
! Cavity radius is calculated from the 1.00 g/cm**3 density.
! FINAL energy is -74.9666740755 after 12 iterations
! Induced dipole= -0.03663, RMS gradient= 0.033467686
!
$contrl scftyp=rhf runtyp=gradient coord=zmt $end
$system memory=300000 $end
$basis gbasis=sto ngauss=3 $end
$guess guess=huckel $end
$scrf radius=1.93 dielec=80.0 $end
$data
water in water, arbitrary geometry
Cnv 2

O
H 1 rOH
H 1 rOH 2 aHOH

rOH = 0.95
aHOH = 104.5
$end
```

```

! EXAM25.
! Illustration of coordinate systems for geometry searches.
! Arbitrary molecule, chosen to illustrate ring, methyl on
! ring, methine H10, imino in ring, methylene in ring.
!
!      H8 H9
!      \|
!      H7-C6 O1---O5 H13
!          \|      \|
!          C2      C4
!          /  \    /  \
!          H10  N3  H12
!              |
!              H11
!
! The initial AM1 energy is -48.6594935
!
!           initial RMS  final E    final RMS  #steps
! Cartesians      0.0200113 -48.7022520  0.0000304   50
! dangling Z-mat  0.0600637 ... OO bond crashes on 1st step
! good Z-matrix   0.0232915 -48.7022510  0.0000285   21
! deloc. coords. 0.0176452 -48.7022537  0.0000267   22
! nat. internals  0.0209442 -48.7022570  0.0000183   15
!
! $contrl scftyp=rhf runtyp=optimize coord=zmt $end
! $system memory=300000 $end
! $statpt hess=guess nstep=100 nprt=-1 npun=-2 $end
! $basis  gbasis=aml $end
! $guess  guess=huckel $end
! $data
! Illustration of coordinate systems
! C1
! O
! C 1 rCOa
! N 2 rCNa 1 aNCO
! C 3 rCNb 2 aCNC 1 wCNCO
! O 4 rCOb 3 aOCN 2 wOCNC
! C 2 rCC 1 aCCO 5 wCCOO
! H 6 rCH1 2 aHCC1 1 wHCCO1
! H 6 rCH2 2 aHCC2 1 wHCCO2
! H 6 rCH3 2 aHCC3 1 wHCCO3
! H 2 rCHa 1 aHCOa 5 wHCOOa
! H 3 rNH 2 aHNC 1 wHNCO
! H 4 rCHb 5 aHCOb 1 wHCOOb
! H 4 rCHc 5 aHCOc 1 wHCOOc
!
! rCOa=1.43
! rCNa=1.47
! rCNb=1.47
! rCOb=1.43
! aNCO=106.0
! aCNC=104.0
! aOCN=106.0
! wCNCO=30.0
! wOCNC=-30.0
! rCC=1.54
! aCCO=110.0
! wCCOO=-150.0
! rCH1=1.09

```

```

rCH2=1.09
rCH3=1.09
aHCC1=109.0
aHCC2=109.0
aHCC3=109.0
wHCCO1=60.0
wHCCO2=-60.0
wHCCO3=180.0
rCHa=1.09
aHCOa=110.0
wHCOOa=100.0
rNH=1.01
aHNC=110.0
wHNCO=170.0
rCHb=1.09
rCHc=1.09
aHCOb=110.0
aHCOc=110.0
wHCOOb=150.0
wHCOOc=-100.0
$end

```

To use Cartesian coordinates:

```
--- $contrl nzvar=0 $end
```

To use conventional Z-matrix, with a dangling O-O bond:

```
--- $contrl nzvar=33 $end
```

To use well chosen internals, with all 5 ring bonds defined:

```
--- $contrl nzvar=33 $end
```

```

--- $zmat  izmat(1)=1,1,2, 1,2,3, 1,3,4, 1,4,5, 1,5,1,
      2,1,2,3, 2,5,4,3, 3,5,1,2,3, 3,1,5,4,3,
      1,6,2, 2,6,2,1, 3,6,2,1,5,
      1,6,7, 1,6,8, 1,6,9, 2,7,6,2, 2,8,6,2, 2,9,6,2,
      3,7,6,2,1, 3,8,6,2,1, 3,9,6,2,1,
      1,10,2, 2,10,2,1, 3,10,2,1,5,
      1,11,3, 2,11,3,2, 3,11,3,2,1,
      1,12,4, 2,12,4,5, 3,12,4,5,1,
      1,13,4, 2,13,4,5, 3,13,4,5,1 $end

```

To use delocalized coordinates:

```
--- $contrl nzvar=33 $end
```

```
--- $zmat  dlc=.true. auto=.true. $end
```

To use natural internal coordinates:

```
$contrl nzvar=44 $end
```

```

$zmat  izmat(1)=1,1,2, 1,2,3, 1,3,4, 1,4,5, 1,5,1,  ! ring !
      2,5,1,2, 2,1,2,3, 2,2,3,4, 2,3,4,5, 2,4,5,1,
      3,5,1,2,3, 3,1,2,3,4, 3,2,3,4,5, 3,3,4,5,1, 3,4,5,1,2,
      1,2,6, 2,6,2,1, 2,6,2,3, 4,6,2,1,3,  ! methyl C !
      1,6,7, 1,6,8, 1,6,9,  ! methyl Hs !
2,7,6,8, 2,8,6,9, 2,9,6,7, 2,9,6,2, 2,7,6,2, 2,8,6,2,
      3,7,6,2,1,
      1,10,2, 2,10,2,1, 2,10,2,3, 2,10,2,6,  ! methine !
      1,11,3, 2,11,3,2, 2,11,3,4, 4,11,3,2,4, ! imino !
      1,12,4, 1,13,4,  ! methylene !
      2,12,4,13, 2,12,4,3, 2,13,4,3, 2,12,4,5, 2,13,4,5

```

```

ijs(1)=1,1, 2,2, 3,3, 4,4, 5,5,           ! ring !
      6,6, 7,6, 8,6, 9,6,10,6,
          7,7, 8,7, 9,7,10,7,
      11,8,12,8,13,8,14,8,15,8,
      11,9,12,9,      14,9,15,9,
          16,10,      17,11,18,11,      19,12,           ! methyl C !
      20,13, 21,14, 22,15,           ! methyl Hs !
      23,16, 24,16, 25,16, 26,16, 27,16, 28,16,
      23,17, 24,17, 25,17,
          24,18, 25,18,
                          26,19, 27,19, 28,19,
                              27,20, 28,20,
      29,21,
          30,22,      31,23,32,23,33,23,      32,24,33,24, ! methine !
          34,25,      35,26,36,26,      37,27,           ! imino !
      38,28, 39,29,           ! methylene !
      40,30, 41,30, 42,30, 43,30, 44,30,
          41,31, 42,31, 43,31, 44,31,
          41,32, 42,32, 43,32, 44,32,
          41,33, 42,33, 43,33, 44,33

Sij(1)=1.0, 1.0, 1.0, 1.0, 1.0,           ! ring !
      1.0, -0.8090, 0.3090, 0.3090, -0.8090,
          -1.1180, 1.8090, -1.8090, 1.1180,
      0.3090, -0.8090, 1.0, -0.8090, 0.3090,
          -1.8090, 1.1180,      -1.1180, 1.8090,
          1.0, 1.0,-1.0, 1.0,           ! methyl C !
      1.0, 1.0, 1.0,           ! methyl Hs !
      1.0, 1.0, 1.0,-1.0,-1.0,-1.0,
      2.0,-1.0,-1.0,
          1.0,-1.0,
                          2.0,-1.0,-1.0,
                              1.0,-1.0,
      1.0,
          1.0,      2.0,-1.0,-1.0,      1.0,-1.0,           ! methine !
          1.0, 1.0,-1.0, 1.0,           ! imino !
      1.0, 1.0,           ! methylene !
      4.0, 1.0, 1.0, 1.0, 1.0,
          1.0,-1.0, 1.0,-1.0,
          1.0, 1.0,-1.0,-1.0,
          1.0,-1.0,-1.0, 1.0      $end

```

```

! EXAM26
! Localized orbital test...see J.Phys.Chem. 1984, 88, 382-389
!
! FINAL Energy= -415.2660357363 in 11 iters
!
! If you localize only the valence orbitals, by commenting
! out the $LOCAL group below, the
!     Boys localization sum is 204.693589
! Ruedenberg localization sum is  5.081667
! population localization sum is  4.610528
!
! The SCF localized charge decomposition forces all orbitals
! to be localized, so the final diagonal sum is 28.389125.
! The nuclear charge assigned to the oxygen "lone pairs" is
! redistributed so that the total nuclear P and O charges are
! correct. The energies computed for the PO bond, PH bonds,
! and O lone pairs are -37.273022, -27.364212, -26.363865.
! The corresponding dipoles are 2.041, 3.484, and 3.465.
!
! To analyze the MP2 valence contributions, select MPLEVEL=2,
! and turn EDCOMP and DIPDCM off. The results should be
! E(MP2)=-415.4952200908, and the contribution of the PO bond,
! PH bonds, and O lone pairs to the correlation energy are
! -0.0442096, -0.0237793, and -0.0378790, respectively.
!
! $contrl scftyp=rhf runtyp=energy local=ruednbrg mplevl=0 $end
! $system memory=750000 $end
! $mp2 lmomp2=.true. $end
! $local edcomp=.true. moidon=.true. dipdcm=.true.
!       ijmo(1)= 1,11, 2,11, 1,12, 2,12, 1,13, 2,13
!       zij(1)=1.6666666667,0.3333333333,1.6666666667,0.3333333333,
!             1.6666666667,0.3333333333
!       moij(1)= 2,1, 2,1, 2,1
!       nnucmo(11)=2,2,2 $end
! $basis gbasis=n21 ngauss=3 ndfunc=1 $end
! $data
! phosphine oxide...3-21G* basis...localized orbital test
! Cnv 3
!
! P 15.0
! O 8.0  0.0000000000  0.0  1.4701
! H 1.0  1.2335928631  0.0  -0.6421021244
! $end

```

```

! EXAM27.
!   NH3   semi-empirical DRC calculation
!
!   The dynamic reaction coordinate is initiated at the
!   planar inversion transition state, with a velocity
!   parallel to the mode with imaginary frequency. The
!   reactive trajectory is given one kcal/mole energy in
!   excess of the amount needed to traverse the barrier.
!   The trajectory is analyzed in terms of the equilibrium
!   geometry's coordinates and normal modes. Because
!   this is a test run, the trajectory is stopped after
!   a much too short time interval.
!
!   The last point on the trajectory has
!   T=0.00163, V=-9.12874, E=-9.12710,
!   q(L6)=-0.153112, p(L6)=-0.014313,
!   velocity(H,z)=0.028857623667
!
$CONTRL SCFTYP=RHF RUNTYP=DRC $END
$SYSTEM MEMORY=300000 $END
$BASIS  GBASIS=AM1 $END
$DATA
ammonia...DRC starting from the planar transition state
C1
NITROGEN   7.0   0.0000000000   0.0000000000   0.0000000000
HYDROGEN   1.0  -0.4882960784   0.8457536168   0.0000000000
HYDROGEN   1.0  -0.4882960784  -0.8457536168   0.0000000000
HYDROGEN   1.0   0.9765921567   0.0000000000   0.0000000000
$END
$DRC NPRTSM=1 NSTEP=10 DELTAT=0.1 NMANAL=.TRUE. EKIN=1.0
      VEL(1)=0.0  0.0  -0.1128,
            0.0  0.0  0.5213,
            0.0  0.0  0.5213,
            0.0  0.0  0.5213
      CO(1)=0.0000000000   0.0000000000   0.0291576578
            -0.4692651161   0.8127910232  -0.3097192193
            -0.4692651161  -0.8127910232  -0.3097192193
            0.9385302321   0.0000000000  -0.3097192193 $END
$HESS
ENERGY IS          -9.1354556210 E(NUC) IS          6.8369847904
 1  1  6.16231432E-01  3.45452916E-11-1.03923982E-05 ...
... 2nd derivatives deleted to save paper ...
12  3  1.38181166E-10  5.72335505E-02
$END

```



```

! EXAM28. Morokuma energy decomposition.
! This run duplicates a result from Table 16 of
! H.Umeyama, K.Morokuma, J.Am.Chem.Soc. 99,1316(1977)
!
!           GAMESS      literature
!      ES=   -14.02     -14.0
!      EX=    8.98       9.0
!      PL=   -1.12     -1.1
!      CT=   -2.37     -2.4
!      MIX=  -0.43     -0.4
!      total -8.96     -9.0
!
! $contrl scftyp=rhf runtyp=morokuma coord=zmt $end
! $system memory=300000 timlim=5 $end
! $basis  gbasis=n31 ngauss=4 $end
! $guess  guess=huckel $end
! $morokm iatm(1)=3 $end
! $data
water-ammonia dimer
Cs

H
O 1 rOH
H 2 rOH 1 aHOH
N 2 R 1 aHOH 3 0.0
H 4 rNH 3 aHNaxis 1 180.0
H 4 rNH 3 aHNaxis 5 +120.0
H 4 rNH 3 aHNaxis 5 -120.0

rOH=0.956
aHOH=105.2
rNH=1.0124
aHNaxis=112.1451 ! makes HNH=106.67
R=2.93
$end

```

```

! EXAM29. surface scan
! The scan is done over a 3x3 grid centered on the SCF
! transition state for the SN2 type reaction
! F- + NH2OH -> F-NH2-OH anion -> FNH2 + OH-
!
! Groups 1 and 2 are F and OH, and their distance from
! the N is varied antisymmetrically, which is more or
! less what the IRC should be like. The results seem to
! indicate that the MP2/3-21G saddle point would shift
! further into the product channel, since the higher
! MP2 energies occur at shorter r(NF) and longer r(NO):
!
! FINAL E= -229.0368324615, E(MP2)= -229.3873302375
! FINAL E= -229.0356378402, E(MP2)= -229.3866642673
! FINAL E= -229.0309266321, E(MP2)= -229.3822094777
! FINAL E= -229.0372146702, E(MP2)= -229.3923234074
! FINAL E= -229.0385440296, E(MP2)= -229.3936486644
! FINAL E= -229.0367369562, E(MP2)= -229.3913683073
! FINAL E= -229.0328601144, E(MP2)= -229.3918932009
! FINAL E= -229.0364643934, E(MP2)= -229.3948325500
! FINAL E= -229.0372478250, E(MP2)= -229.3943498144
!
! A more conclusive way to tell this would be to compute
! single point MP2 energies along the SCF IRC, since the
! true reaction path always curves, and thus does not lie
! along rectangular grid points.
!
$contrl scftyp=rhf runtyp=surface
        icharg=-1 coord=zmt mplevl=2 $end
$system memory=500000 timlim=30 memddi=2 $end
$surf  ivec1(1)=2,1 igrp1=1
        ivec2(1)=2,5 igrp2(1)=5,6
        displ= 0.10 ndisp1=3 orig1=-0.10
        disp2=-0.10 ndisp2=3 orig2= 0.10 $end
$basis  gbasis=n21 ngauss=3 $end
$guess  guess=huckel $end
$data
F-NH2-OH exchange (inspired by J.Phys.Chem. 1994,98,7942-4)
Cs

F
N 1 rNF
H 2 rNH 1 aFNH
H 2 rNH 1 aFNH 3 aHNH +1
O 2 rNO 3 aONH 4 aONH -1
H 5 rOH 2 aHON 1 180.0

rNF=1.7125469
rNH=0.9966981
rNO=1.9359887
rOH=0.9828978
aFNH=90.18493
aONH=79.34339
aHON=100.78851
aHNH=108.57000
$end

```

```

!   EXAM30
!   Test of water EFP ... formamide/three water complex
!
!   FINAL E= -169.0085352303 after 12 iterations
!   RMS gradient=0.008099469
!
!   The geometry below combines a computed gas phase
!   structure for formamide, with three waters located
!   in a cyclic fashion whose positions approximate the
!   minimum structure of W.Chen and M.S.Gordon. This
!   approximate structure lies about 11 mHartree above
!   the actual minimum.
!
!   $contrl scftyp=rhf runtyp=gradient coord=zmt $end
!   $system memory=300000 $end
!   $basis  gbasis=dh npfunc=1 ndfunc=1 $end
!   $data
formamide with three effective fragment waters
C1
C
O 1 rCO
N 1 rCN  2 aNCO
H 3 rNHa 1 aCNHa 2 0.0
H 3 rNHb 1 aCNHb 2 180.0
H 1 rCH  2 aHCO  4 180.0

rCO=1.1962565
rCN=1.3534065
rNHa=0.9948420
rNHb=0.9921367
rCH=1.0918368
aNCO=124.93384
aCNHa=119.16000
aCNHb=121.22477
aHCO=122.30822
$end
$efrag
coord=int
fragname=H2Oef2
O1  4 1.926      3 175.0      1 180.0
H2  7 0.9438636  4 117.4      3 -175.0
H3  7 0.9438636  8 106.70327  4 95.0
fragname=H2Oef2
O1  8 1.901      7 175.0      4 0.0
H2 10 0.9438636  8 110.0      4 -5.0
H3 10 0.9438636 11 106.70327  8 -95.0
fragname=H2Oef2
H2  2 1.951      1 150.0      3 0.0
O1 13 0.9438636  2 177.0      3 0.0
H3 14 0.9438636 13 106.70327  3 140.0
$end

```

```

! EXAM31.
! Water in PCM water...RHF geometry optimization
!
! FINAL E= -74.9677081860, 12 iters, RMS GRAD = 0.0321490
! FINAL E= -74.9494679452, 8 iters, RMS GRAD = 0.0647800
! FINAL E= -74.9690975801, 7 iters, RMS GRAD = 0.0238593
! FINAL E= -74.9712684509, 7 iters, RMS GRAD = 0.0081236
! FINAL E= -74.9715453381, 8 iters, RMS GRAD = 0.0018667
! FINAL E= -74.9714737628, 7 iters, RMS GRAD = 0.0049760
! FINAL E= -74.9715558829, 7 iters, RMS GRAD = 0.0000526
! FINAL E= -74.9715559513, 4 iters, RMS GRAD = 0.0000260
!
! The final geometry is not symmetric,
! O
! H 1 .9873716
! H 1 .9872902 2 100.0327788
!
! -----
! ----- RESULTS OF PCM CALCULATION -----
! -----
!
! FREE ENERGY IN SOLVENT = -74.9715559513 A.U.
! INTERNAL ENERGY IN SOLVENT = -74.9655730812 A.U.
! DELTA INTERNAL ENERGY = .0000000000 A.U.
! ELECTROSTATIC INTERACTION = -.0059828701 A.U.
! PIEROTTI CAVITATION ENERGY = .0000000000 A.U.
! DISPERSION FREE ENERGY = .0000000000 A.U.
! REPULSION FREE ENERGY = .0000000000 A.U.
! TOTAL INTERACTION = -.0059828701 A.U.
! TOTAL FREE ENERGY IN SOLVENT = -74.9715559513 A.U.
!
! $contrl scftyp=rhf runtyp=optimize coord=zmt $end
! $system memory=300000 $end
! $basis gbasis=sto ngauss=3 $end
! $guess guess=huckel $end
! $pcm solvnt=water $end
! $data
a water molecule solvated by PCM water
Cnv 2
O
H 1 rOH
H 1 rOH 2 aHOH
rOH=0.95
aHOH=104.5
$end

```