(6 May 2012)

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* Section 3 - Input Examples *
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The GAMESS distribution contains a number of short input examples:

a) in a source code distribution, see
~/gamess/tests/standard/exam*.inp

b) in a binary distribution for Apple Macintosh, see
~/gamess/tests/standard/exam*.inp

c) in a binary distribution for Windows, see
C:\gamess.64\tests\exam*.inp (or C:\gamess.32)

Please see the summary table below to note what kinds of calculations are included.

The primary usage of these input files is to introduce the basic functionality of the program. Running all of these, and noting where in the log file the key results contained in comments in the input files appear should introduce the basics to a new user. After that, explore the more exotic keywords in the previous chapter, for the number of examples in the test packet is deliberately kept small, and each run is relatively simple.

Secondarily, running these tests serves as a simplistic verification of the program's correct installation. In source code distributions, only, there is a script to check the numerical results, see
~/gamess/tests/standard/checktst
to automatically check all results. Binary distributions can do this by hand, since the expected results are contained in the input files. Note that to keep the tests small, the memory and CPU time required is trivially small. This means that problems that might occur in larger runs won't be detected, and that these tests are entirely inappropriate for parallel execution.

The examples are:

| Example | Description |
|---|---|
| 1 | CH2 RHF geometry optimization |
| 2 | CH2 UHF + gradient |
| 3 | CH2 ROHF + gradient |
| 4 | CH2 GVB + gradient |

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     5          CH2 RHF + CI gradient
     6          CH2 MCSCF geometry optimization
     7          HPO RHF + gradient
     8          H2O RHF + MP2 gradient
     9          H2O MCSCF + MCQDPT energy correction
    10          H2O RHF + hessian (vibrational analysis)
    11          HCN RHF Intrinsic Reaction Coordinate
    12         HCCH closed shell DFT geometry opt.
    13          H2O RHF properties
    14          H2O CI transition moment
    15          C2- GVB/ROHF on 2-pi-u state
    16           Si GVB/ROHF on 3-P state
    17          CH2 GVB/ROHF + hessian
    18           P2 RHF + hessian, effective core pot.
    19           NH spin-orbit coupling
    20           I- exponent TRUDGE optimization
    21        CH+H2 open shell TCSCF hessian
    22         H3CN UHF + UMP2 gradient
    23        SiH3- PM3 geometry optimization
    24          H2O SCRF test case
    25            ? internal coordinate example
    26         H3PO localized orbital test
    27          NH3 Dynamic Reaction Coordinate (ie, AIMD)
    28      H2O-NH3 Morokuma/Kitaura energy decomposition
    29       FNH2OH simple potential surface scan
    30 HCONH2(H2O)3 effective fragment potential solvation
    31        CH3OH PCM test case
    32          HNO coupled cluster test
    33          HCN ORMAS-MCSCF illustration
    34         H2CO CIS optimization
    35           As relativity via Douglas-Kroll
    36         C2H4 MCSCF analytic hessian
    37       (H2O)3 Fragment Molecular Orbital RHF
    38         AsH3 model core potential geometry opt.
    39          CH4 Raman and hyper-Raman spectra
    40          CH2 minimum energy crossing point search
    41           CO TDDFT excitation energy/gradient
    42           CN open shell CC numerical gradient
    43          CH4 heat of formation
    44        (HF)6 divide-and-conquer MP2 energy
    45          CH2 closed shell EOM-CCSD plus triples
    46          NH2 open shell EOM-CCSD
    47          Cl- ionization potential by IP-EOM3a

The following will refuse to run in parallel:
   5 - CI gradient is not enabled for parallel execution
   23,25,27 - MOPAC is not enabled for parallel execution
   32,42,45,46,47 - only RHF-based CCSD/CCSD(T) is parallel
   39 - RUNTYP=TDHFX is not enabled for parallel execution
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