

(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

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~/gamess/tests/standard/checktst
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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

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The following will refuse to run in parallel:

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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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