

Basic Setup | **Advanced Setup**

- Basis
- Control
 - SCF
 - DFT
 - Data**
- System
- MO Guess
- Misc

Title:

Coordinate Type:

Units:

Point Group:

of Z-Matrix Variables:

Order of Principal Axis:

Use Symmetry During Calculation

! File created by the GAMESS Input Deck Generator Plugin for Avogadro

\$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.TRUE. **\$END**

\$CONTRL SCFTYP=RHF RUNTYP=ENERGY DFTTYP=B3LYP **\$END**

\$DATA

Title

C1

| | | | | |
|---|-----|----------|----------|----------|
| C | 6.0 | 0.00000 | -0.00000 | 0.00000 |
| H | 1.0 | 0.00000 | -0.89000 | -0.62930 |
| H | 1.0 | 0.00000 | 0.89000 | -0.62930 |
| H | 1.0 | -0.89000 | -0.00000 | 0.62930 |
| H | 1.0 | 0.89000 | -0.00000 | 0.62930 |

\$END

Reset All

Defaults

Compute...

Generate...

Close