Cheat-Sheat for `tools-for-g16.bash`
(0.0.14, 2018-08-20)
Martin C Schwarzer, September 4, 2018

Introduction

This accompanies the repository polyluxus/tools-for-g16.bash.

Various bash scripts to aid the use of the quantum chemistry software package Gaussian 16.

`g16.prepare.sh`

`g16.testroute.sh`

`g16.freqinput.sh`

`g16.submit.sh`

`g16.getenergy.sh`

`g16.getfreq.sh`

`g16.chk2xyz.sh`

`-m <ARG>` Memory

Author, Bugs, and the Rest

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