



G3:M1:V1 - Gaussian Calculation Setup

Title: **Title Card Required**

Keywords: **# opt freq uapfd/6-311++g(2d,p) geom=connectivity**

Charge/Mult.: **0 1**

Job Type Method Title Link 0 General Guess Pop. PBC Solvation Add. Inp. Preview

☐ Multilayer ONIOM Model

Method: Ground State DFT... Unrestricted APFD

Basis Set: 6-311G ++ (2d , p)

Charge: 0 Spin: Singlet

☐ Use sparse matrices

Additional Keywords: Update

Scheme: (Unnamed Scheme) Assign to Molecule Group

Submit... Quick Launch Cancel Edit... Retain Defaults

G3:M1:V1 - acetoneSubmit.gif (C:/Users/user5/Przemyslaw Dzieńisiewicz/acetoneSubmit.gif)

10 atoms, 32 electrons, neutral, singlet

To samo się dzieje, ktoś musiał odpalić wcześniej

Łaci: dziękuję

MC DL