

GAMESS calculations in parallel environment

Svajonė VOŠTERIENĖ (KA), Juozas ŠULSKUS (VU)

e-mail: svajone.vosteriene@lka.lt, juozas.sulskus@ff.vu.lt

1. Introduction

Cluster based on PC's running Linux was created in the Applied Sciences Department in Lithuanian Military Academy. Created computational facilities were applied to investigate electronic structure and vibration spectra of trinitrotoluene molecule by means of nonempirical quantum mechanical computation methods. During investigations the General Atomic and Molecular Electronic Structure System (GAMESS) quantum chemistry computer code was used [1]. The basis of these investigations is quantum mechanics, but in order to achieve quantitative results comparable with experimental we need supercomputer's power or parallel computers cluster. In this work we continue our previous investigations [2,3].

2. Results of trinitrotoluene and 2,4,6-trinitrophenol calculations

Theoretical investigations of trinitrotoluene and 2,4,6-trinitrophenol molecules were performed by means of *ab initio* quantum mechanical methods using GAMESS computer code [1].

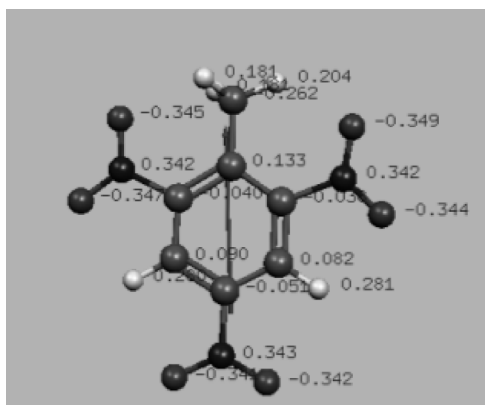


Fig. 1a. Charges of the atoms in TNT molecule (in a.u.) calculated in HF approximation in the 6-311G (1d, 1f, 1p) basis set. Arrows show approximate direction of the dipole moment ($D_{HF} = 4,005D$).

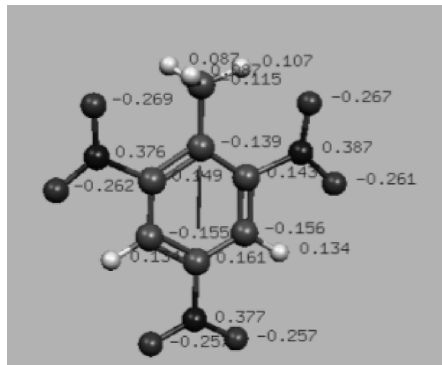


Fig. 1b. Charges of the atoms in TNT molecule (in a.u.) calculated in HF+MP2 approximation in the 6-311G (2d, 2p) basis set. Arrows show approximate direction of the dipole moment ($D_{HF} = 1, 303D$).

Table 1. Geometry optimization results and necessary CPU time dependence from basis set used (number of basis functions). Computations were performed in HF approximation

Basis set	Numb. of basis functions	$E_{tot.HF} + 880, a.u.$	Dipole moment, D	Computational time, min.(h)
6-31G(1d)	250	-0.11701925	1.7586	146.9 (2.45)
6-311G(2d)	415	-0.36559238	1.7020	555.0 (9.25)
6-311G(3d+1f)	671	-0.42604909	1.7277	5349.8 (89.16)

Basis set 6-311G (with polarization d functions on second period elements) was used. All in all for trinitrotoluene we had 250 and for 2,4,6-trinitrophenol 246 basis functions. During multiconfigurational selfconsistent field (MCSCF) [4] calculations performed for trinitrotoluene we left unfrozen 10 highest occupied MO and 10 lowest unoccupied MO from Hartree-Fock Slater determinant. All configurations generated from unfrozen MO's with spin projection zero were included in MCSCF procedure. We had more than 65000 configurations. All unfrozen MO's are orbital of benzene ring and NO_2 groups. Full geometry optimization was performed for trinitrotoluene molecule in Hartree-Fock and in MCSCF approximations and in HF approximation for 2,4,6-trinitrophenol molecule. Even with such comparatively small cluster we can perform all necessary computations at HF level.

3. The influence of NO_2 groups to electronic structure of nitrotoluene compounds

2,4,6-trinitrotoluene is better known by its initials, TNT. It is an important explosive, since it can very quickly change from a solid into hot expanding gases. TNT have 3 NO_2 groups (from nitric acid) to toluene. TNT is explosive for two reasons. First, it

contains the elements carbon, oxygen and nitrogen, which means that when the material burns it produces highly stable substances (CO , CO_2 and N_2) with strong bonds, so releasing a great deal of energy. The number of NO_2 groups influence the electronic structure and vibration spectra of molecule. Theoretical investigations of molecules with two and one NO_2 groups were performed by means of *ab initio* quantum mechanical methods using GAMESS computer code [1]. Basis set 6-311G with polarization functions (2d,2p; 1d,1f,1d; 3d,1f,3p) was used. Full geometry optimization was performed in Hartree-Fock approximation with MP2 energy analysis. The results of stability of NT and DNT is shown in Figs. 2, 3.

Calculations let us to know necessary resources of cluster for investigations (Table 2).

For this calculations was assume that we will used the SMP2 personal computers. For each node GAMESS computer code [1] execute two tasks and this means that for one CPU we need about 1 GB RAM. The important feature of the our cluster that it may be upgraded or expanded without any essential rebuilds.

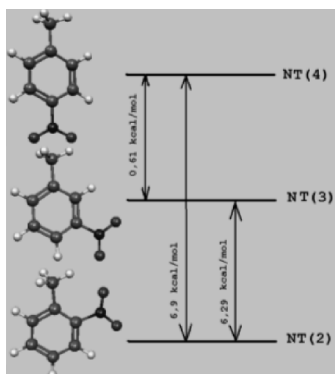


Fig. 2. Stability of NT molecule calculated in HF approximation in the 6-311G (3d.1f.3p) basis set.

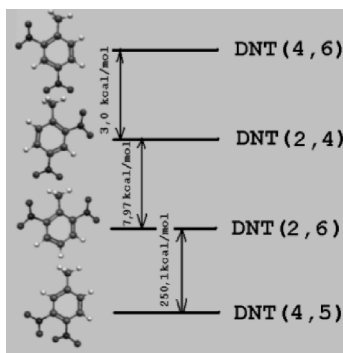


Fig. 3. Stability of DNT molecule calculated in HF approximation in the 6-311G (3d.1f.3p) basis set.

Table 2. Necessary resources for computations performed in HF+MP2 approximation

Basis set	Number of basis functions	Approximation	Necessary RAM in MB	Necessary nodes with 2GB RAM
6-311G(3d,1f,3p)	716	HF + MP2	7 320	4
6-311G(3d,1f,3p)+diffsp,+diffs	785	HF + MP2	8 776	5
TZV (3d,1f,3p)	732	HF + MP2	7648	5
TZV(3d,1f,3p)+diffsp,+diffs	801	HF + MP2	9128	6

4. Conclusions

Created PCs cluster allows solving of modern quantum chemical problems at necessary level. Trinitrotoluene molecule calculations by MCSCF method show significant change of vibrational spectrum characteristics from those calculated at Hartree-Fock level. Achieved results allow more detail interpretation of experimental vibrational spectra of investigated molecules and more accurate investigation of thermochemical reactions dynamics.

The precise knowledge of vibrational spectra would allow detecting small amounts of these materials by means of spectroscopic methods. It concerned with the possibility to apply spectroscopic methods for solving of ecological and monitoring problems.

References

1. A.A. Granovsky. [wwwhttp://classic.chem.msu.su/gran/gamess/index.html](http://classic.chem.msu.su/gran/gamess/index.html).
2. S. Cicenenas, R.J. Rakauskas, S. Vošterienė, J. Šulskus, Theoretical investigation of the vibrational spectra of trinitrotoluene and 2,4,6-trinitrophenol molecules, *Lithuanian Journal of Physics*, **41**, 221–224 (2001).
3. R.J. Rakauskas, J. Šulskus, S. Vošterienė, PC cluster possibilities in mathematical modeling in quantum mechanical molecular computations, *Nonlinear Analysis: Modelling and Control*, **7**, 113–121 (2002).
4. M.W. Schmidt, M.S. Gordon, The construction and interpretation of MCSCF wavefunctions, *Ann. Rev. Phys. Chem. V.*, **49**, 233 (1998).
5. M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, J.A. Montgomery, Jr., The general atomic and molecular electronic structure system, *J. Comput. Chem.*, **14**, 1347 (1993).
6. W. Gropp, E. Lusk, A. Skjellum, *Using MPI*, The MIT Press (1999).
7. <http://clusters.top500.org/db>

REZIUOMĖ

S. Vošterienė, J. Šulskus. Gamess paketo taikymai lygiagrečiųjų skaičiavimų architektūroje

Lietuvos Karo Akademijos Taikomųjų mokslų katedros mokomosios kompiuterių klasės bazėje buvo sukurtas lygiagrečiųjų skaičiavimų kompiuteris. Sukurtas kompiuteris buvo panaudotas tirti teršalų molekulių elektroninei struktūrai bei vibracinių spektrų tyrimui kvantinės mechanikos skaičiavimo programa Gamess. Gauti preliminarūs trinitrotoluolo molekulės harmoniniai vibraciniai spektrai Hartrio ir Foko artinyje. Ištirta galimybė skaičiuoti tiriamų molekulių vibracinius spektrus patikslintaisiais metodais bei atsižvelgiant į anharmonizmą.