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calculations and Optimizing molecule  
using Gaussian software قييفيك

دوانرب رادختسرا Gaussian 09 ( قودقور )

Example of Thermochemistry  
Calculation in Gaussian 09

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~~Notes~~  
~~in Gaussian~~ Gaussian scans

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What is Gaussian Noise? Molecular  
Optimization and Frequency  
Calculation: Gaussian Grignard  
~~Reaction (Transition State) Gaussian~~  
~~09~~ Optimizing Transition State of SN2  
Reaction (Gaussian) How to Scan a  
Dihedral in Gaussian GaussView 6

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**Tutorial 4: 3-D Results Visualization**  
How to perform and analyze NMR  
DFT calculations in GaussView and  
Gaussian Calculating UV-Vis and  
electronic circular dichroism (ECD)  
spectra of HFCIC-CHFOH and ClFHC-  
CHFOH. Result Analysis: Gaussian  
Performing a Relaxed Coordinate

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Notes  
Scan with Gaussian and GaussView  
How to draw HOMO and LUMO  
orbitals in GaussView using Gaussian  
output file

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How to calculate Fukui functions and  
Global reactivity parameters using  
Gaussian software

~~How to do TD-DFT  
Calculations (UV calculations) using~~



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~~GaussView and Gaussian software~~  
1:00 PM - Air Force 2019 X \u0026amp; Y  
Group | English by Sanjeev Sir | 25  
Questions with Detailed Solution 16-  
Kondo effect and numerical  
renormalization group - Course on  
Quantum Many-Body Physics Design  
Theories | Reinforced Cement

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Concrete | Lec 7 | SSC JE Civil  
Engineering Book 1 Lesson 17  
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Processes : Introduction to Random  
Process Gaussian 09 Revision E 01  
Frisch, M., et al. (2009) Gaussian 09.  
Revision E.01, Gaussian Inc.,  
Wallingford CT. has been cited by the

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following article: TITLE: Rylene  
Dielectrophores for Capacitive Energy  
Storage. AUTHORS: Andrey  
Borzenko, Carine Edder, Lev  
Mourokh, Pavel Lazarev.  
KEYWORDS: Dielectrophore,  
Polarization, Capacitor, Molecular  
Dielectrics, Molecular Design

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Frisch, M., et al. (2009) Gaussian 09.  
Revision E.01 ...

\*Feature and Usage notes: Rev E.01  
This revision is primarily to fix a variety  
of bugs reported by users or which  
were uncovered by the example jobs  
for the 3rd edition of Exploring

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Notes  
Chemistry with Electronic Structure  
Methods.

Gaussian 09 Revision E.01 Release  
Notes

Gaussian 09, Revision E.01, Frisch,  
M. J., Trucks, G. W., Schlegel, H. B.,  
Scuseria, G. E., Robb, M. A.,

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Notes  
Cheeseman, J. R., Scalmani, G.,  
Barone, V., Mennucci, B ...

Gaussian 09, Revision E.01, Frisch,  
M. J., Trucks, G. W ...

Gaussian 09, Revision E.01, M. J.  
Frisch, G. W. Trucks, H. B. Schlegel,  
G. E. Scuseria, M. A. Robb, J. R.

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Notes  
Cheeseman, G. Scalmani, V. Barone,  
B. Mennucci, G. A. Petersson, H.  
Nakatsuji, M. Caricato, X. Li, H. P.  
Hratchian, A. F. Izmaylov, J. Bloino, G.  
Zheng, J. L. Sonnenberg, M. Hada, M.  
Ehara, K. Toyota, R. Fukuda, J.  
Hasegawa, M. Ishida, T. Nakajima, Y.  
Honda, O. Kitao, H. Nakai, T. Vreven,

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J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin ...

## Gaussian 09 Citation

In some cases, Gaussian output will display the references relevant to the current calculation type. Gaussian also



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Includes the NBO program as link 607.  
If this program is used, it should be  
cited separately as: NBO Version 3.1,  
E. D. Glendening, A. E. Reed, J. E.  
Carpenter, and F. Weinhold.

Gaussian 09 Citation | Gaussian.com  
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Frisch and others published Gaussian

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**Notes** for Source Code Version (see also notes above):. In order to build on Intel-based Macintosh computers, the source code and tools must be installed on an HFS+ case-sensitive file system (or a UFS file system for systems where that is supported).; Fujitsu SPARC64 builds the utilities

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Notes  
gau-machine, gau-cpp and gau-fsplit

...

Revision C.01 | Gaussian.com

Last updated on: 23 July 2019. Quick  
Links. Basis Sets; Density Functional  
(DFT) Methods; Solvents List SCRF

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Citation | Gaussian.com

Frisch, M. J. et al., Gaussian 03, revision E. 01, Gaussian Inc., Wallingford CT, 2004. has been cited by the following article: Article. Modeling of Ionization Energy of Elements Using Hartree-Fock Method: An Introduction to Computational

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Notes  
Quantum Chemistry for  
Undergraduate Students.

Frisch, M. J. et al., Gaussian 03,  
revision E. 01 ...

Changes Between Gaussian 16 and  
Gaussian 09; CIS; Citation; Citation;  
DFT Functionals Double Hybrid;



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External; G16W System  
Requirements; Gaussian 16  
Frequently Asked Questions;  
Gaussian 16 Rev. A.03 Release  
Notes; Gaussian 16 Rev. B.01  
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Frisch, M.J., et al. (2009) Gaussian 09, Revision B. 01. Gaussian, Inc., Wallingford. has been cited by the following article: TITLE: Spectroscopic

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Evaluation of the Molecular Structures  
of di- $\mu$ -Chlorobis(1,5-Cyclooctadiene)  
Iridium (I) and Rhodium (I) Complexes.  
AUTHORS: Saheed A. Popoola,  
Abdulaziz A. Al-Saadi

Frisch, M.J., et al. (2009) Gaussian 09,  
Revision B. 01 ...

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Frisch, M.J., Trucks, G.W., Schlegel, H.B., et al. (2016) Gaussian 09 Revision E.01. Gaussian Inc., Wallingford.

Frisch, M.J., Trucks, G.W., Schlegel, H.B., et al. (2016 ...  
The optimized Cartesian coordinates



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of stationary points for the reaction 1 +  
CH<sub>3</sub>COOBr with the SCRF-  
B3LYP/6-31G\* method in water with  
the Gaussian 09 program package.  
Table S2.

I am trying to generate a wfx file by  
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**Notes** The current required citation for Gaussian 03 is the following (presented here in three formats for convenient cutting and pasting). Note that this is an updated list with respect to that printed out by earlier revisions of the program, but it applies to every revision of Gaussian 03.. Normal

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