東京大学　生産技術研究所
北條　博彦

化学生命工学専攻

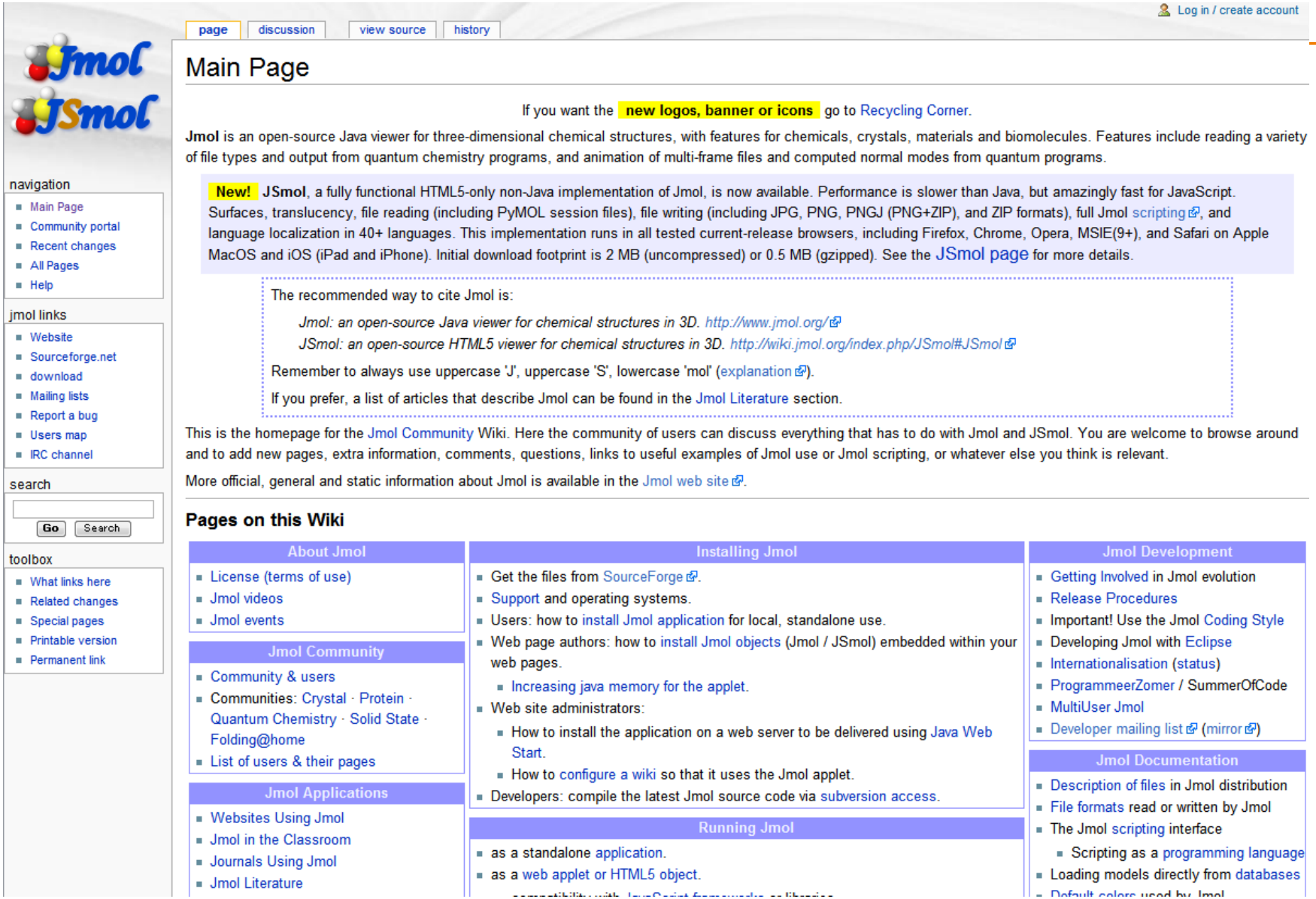
有機機能材料学特論II

分子構造の表現法

原子位置のデータ
- デカルト座標系
- 分率座標系
- 内部座標系

分子構造の描画
- wireframe（線画）
- ball&stick（豆細工模型, boll&stickとも）
- CPK（Corey-Pauling-Kultun）
- ORTEP
- helix, sheet, ribbon

http://wiki.jmol.org/index.php/Main_Page



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Main Page

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JSmol: an open-source HTML5 viewer for chemical structures in 3D. http://wiki.jmol.org/index.php/JSmol#JSmol

Remember to always use uppercase 'J', uppercase 'S', lowercase 'mol' (explanation).

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This is the homepage for the Jmol Community Wiki. Here the community of users can discuss everything that has to do with Jmol and JSmol. You are welcome to browse around and to add new pages, extra information, comments, questions, links to useful examples of Jmol use or Jmol scripting, or whatever else you think is relevant.

More official, general and static information about Jmol is available in the Jmol web site.

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- List of users & their pages

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Installing Jmol
- Get the files from SourceForge.
- Support and operating systems.
- Users: how to install Jmol application for local, standalone use.
- Web page authors: how to install Jmol objects (Jmol / JSmol) embedded within your web pages.
  - Increasing java memory for the applet.
- Web site administrators:
  - How to install the application on a web server to be delivered using Java Web Start.
  - How to configure a wiki so that it uses the Jmol applet.
- Developers: compile the latest Jmol source code via subversion access.

Running Jmol
- as a standalone application.
- as a web applet or HTML5 object.

Jmol Development
- Getting Involved in Jmol evolution
- Release Procedures
- Important! Use the Jmol Coding Style
- Developing Jmol with Eclipse
- Internationalisation (status)
- ProgrammeerZomer / SummerOfCode
- MultiUser Jmol
- Developer mailing list (mirror)

Jmol Documentation
- Description of files in Jmol distribution
- File formats read or written by Jmol
- The Jmol scripting interface
  - Scripting as a programming language
- Loading models directly from databases

Jmol Documentation and Examples

interactive script documentation
what's new in Jmol 11.4 and what's in development for Jmol 11.6 -- Change Log.
Jmol Version 10 examples
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Jmol Files and Code

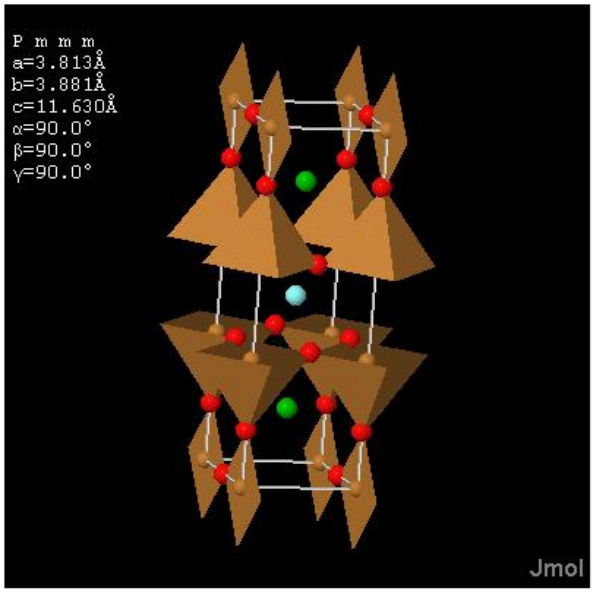
Jmol SourceForge Development Page
Hanson's latest bleeding edge ZIP file (Jmol 11.3)
very latest JAR files and example directory
Jmol subversion repository branch for version 11.2
Jmol subversion repository trunk (version 11.3)
Preliminary JVXL file format documentation

Jmol Ajax/On-Demand JavaScript Examples

simple ajax example GoogleIndex "on-demand JavaScript" example Clickable "on-demand JavaScript" example
XTALX Jmol Crystal Explorer

Jmol Presentations (not necessarily self-guided)

Peter Murray-Rust: The Semantic Chemical Web: GoogleInChI and other Mashups
Spring 2006 ConfChem paper
August 2006 Cologne/Nijmegen seminar (requires PC/LiveWeb)
BCCE19 Ajax for Chemistry
(requires Windows PC/Microsoft PowerPoint with LiveWeb add-in)



PDB alternate locations
crystallographic symmetry
dipoles
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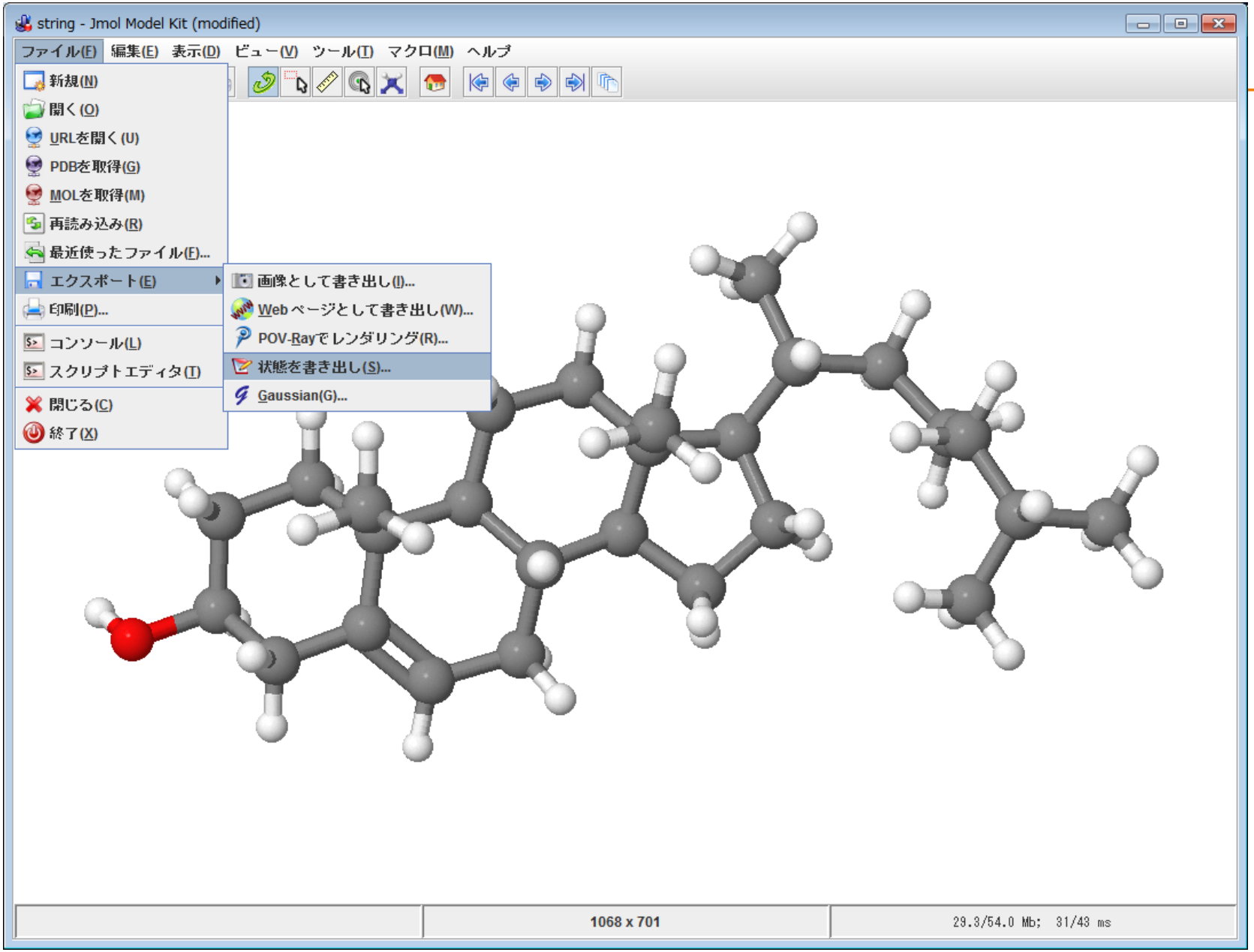
measurements
molecular orbitals
pmesh inline
polyhedra
reading vibration data
Molecular Origami of zircon


string - Jmol Model Kit (modified)
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編集(E)
表示(D)
ビュー(V)
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マクロ(M)
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Gaussian(G)...
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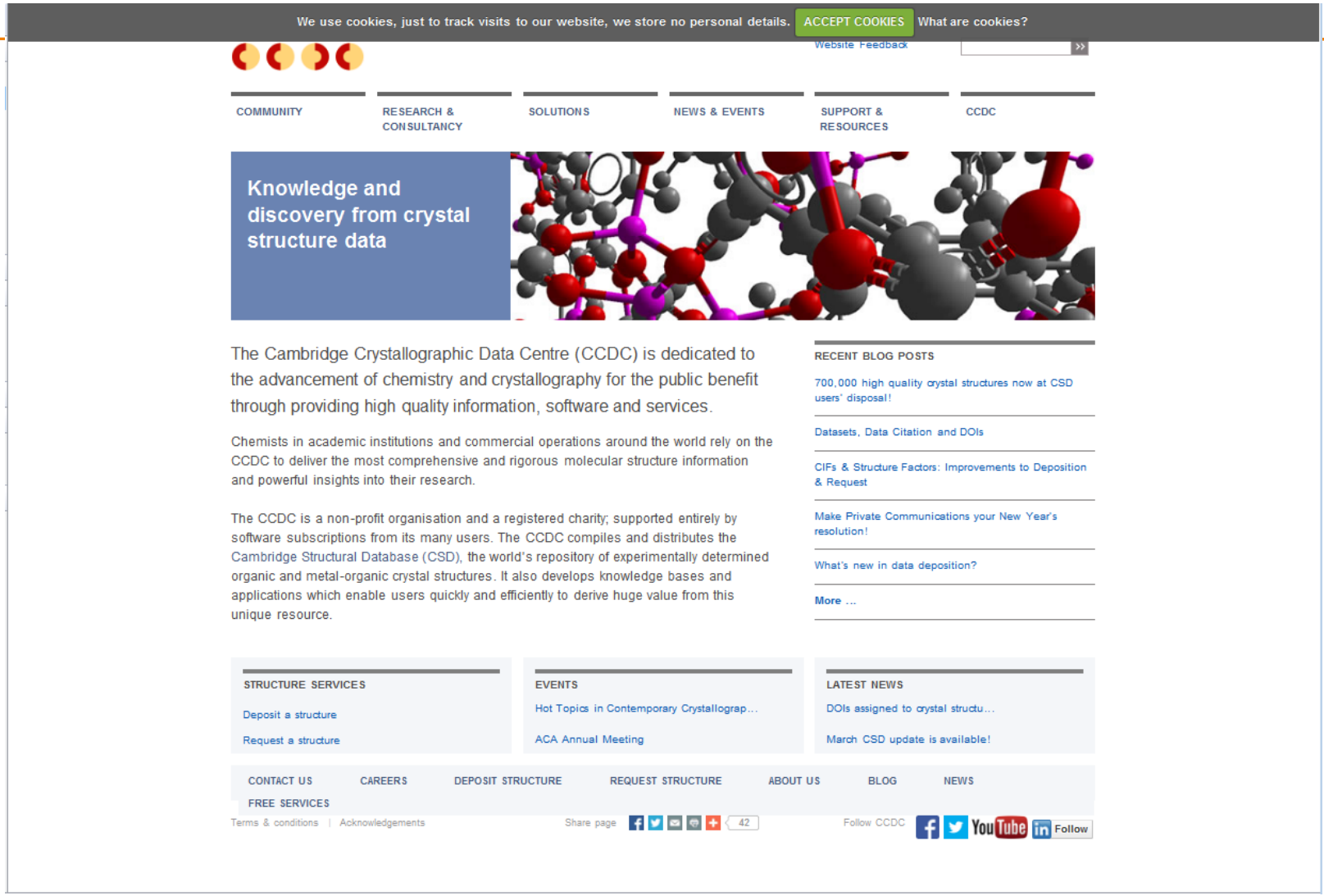
http://www.ccdc.cam.ac.uk/pages/Home.aspx



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Publications

Bulletin of the Chemical Society of Japan (2013), 86, 698, doi:10.1246/bcsj.20120316 Hajime Shingai, Hirohiko Houjou, Isao Yoshikawa, Koji Araki

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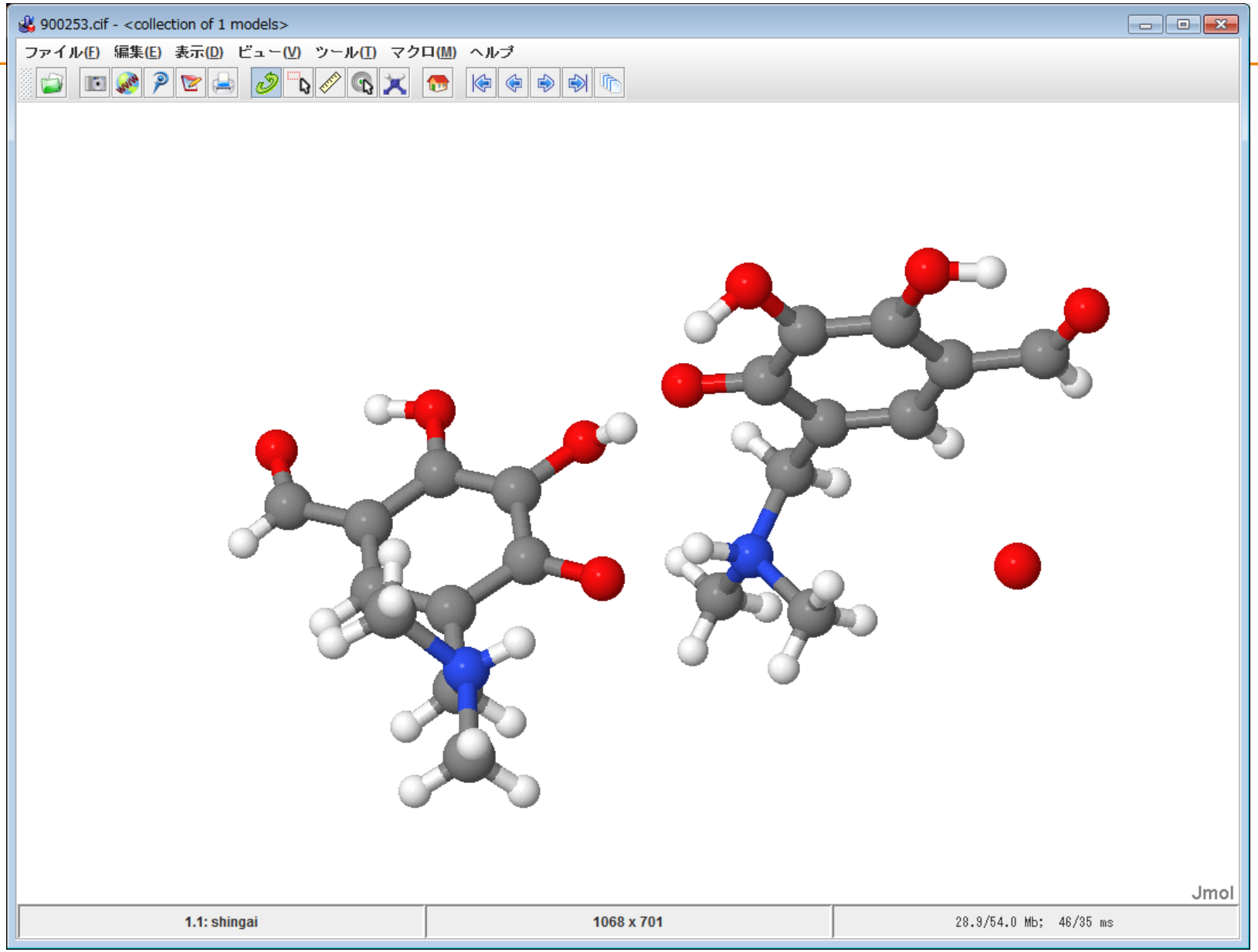
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28.9/54.0 Mb; 46/35 ms

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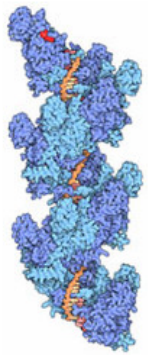
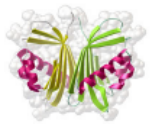


Molecule of the Month

RecA and Rad51

Breakage of DNA is bad news, so cells have powerful methods to fix damaged DNA. One method trims the broken ends and then reconnects them back together. This is fast and easy, but has the disadvantage of possibly incorporating errors during the repair. Cells also have a more accurate method to repair breaks that relies on duplicate copies of the genome. This process is called homologous recombination, and rebuilds the damaged areas using an intact copy as a template.

Full Article



Protein Structure Initiative Featured System

New NTF2-like Domains

The orderly nature of protein folding was one of the great surprises of the early days of structural biology. As more and more protein structures were solved, structural biologists discovered that there are a finite number of ways that a protein chain can fold into a stable structure. One of the goals of PSI researchers has been to enumerate these possible folds, and to understand how they are morphed through evolution to perform many different cellular tasks.

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Structure of the Phosphopantetheine Transferase Sfp in Complex with Coenzyme A and a Peptidyl Carrier Protein

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- mmCIF File (gz)
- PDBML/XML File
- PDBML/XML File (gz)
- Structure Factor (Text)
- Structure Factor (gz)
- Biological Assembly (gz) (A+S)

DOI: 10.2210/pdb4mrt/pdb

Primary Citation

Crystal Structure of a PCP/Sfp Complex Reveals the Structural Basis for Carrier Protein Posttranslational Modification.

Tufar, P., Rahighi, S., Kraas, F.I., Kirchner, D.K., Lohr, F., Henrich, E., Kopke, J., Dikic, I., Guntert, P., Marahiel, M.A., Dotsch, V.

Journal: (2014) Chem.Biol.

PubMed: 24704508
DOI: 10.1016/j.chembiol.2014.02.014
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Phosphopantetheine transferases represent a class of enzymes found throughout all forms of life. From a structural point of view, they are subdivided into three groups, with transferases from group II being the most widespread. They are required for the posttranslational...
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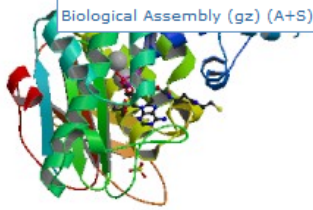
Molecular Description Hide

Classification: Transport Protein/transferase
Structure Weight: 38222.83

Molecule: Tyrocidine synthase 3
Polymer: 1 **Type:** protein **Length:** 90
Chains: C
Fragment: Peptidyl carrier protein domain(UNP Residues 3038-3113)
Mutation: S3075A
Organism Brevibacillus parabrevis
Gene Name tycC
UniProtKB: Protein Feature View | Search PDB | O30409



3D View More Images...

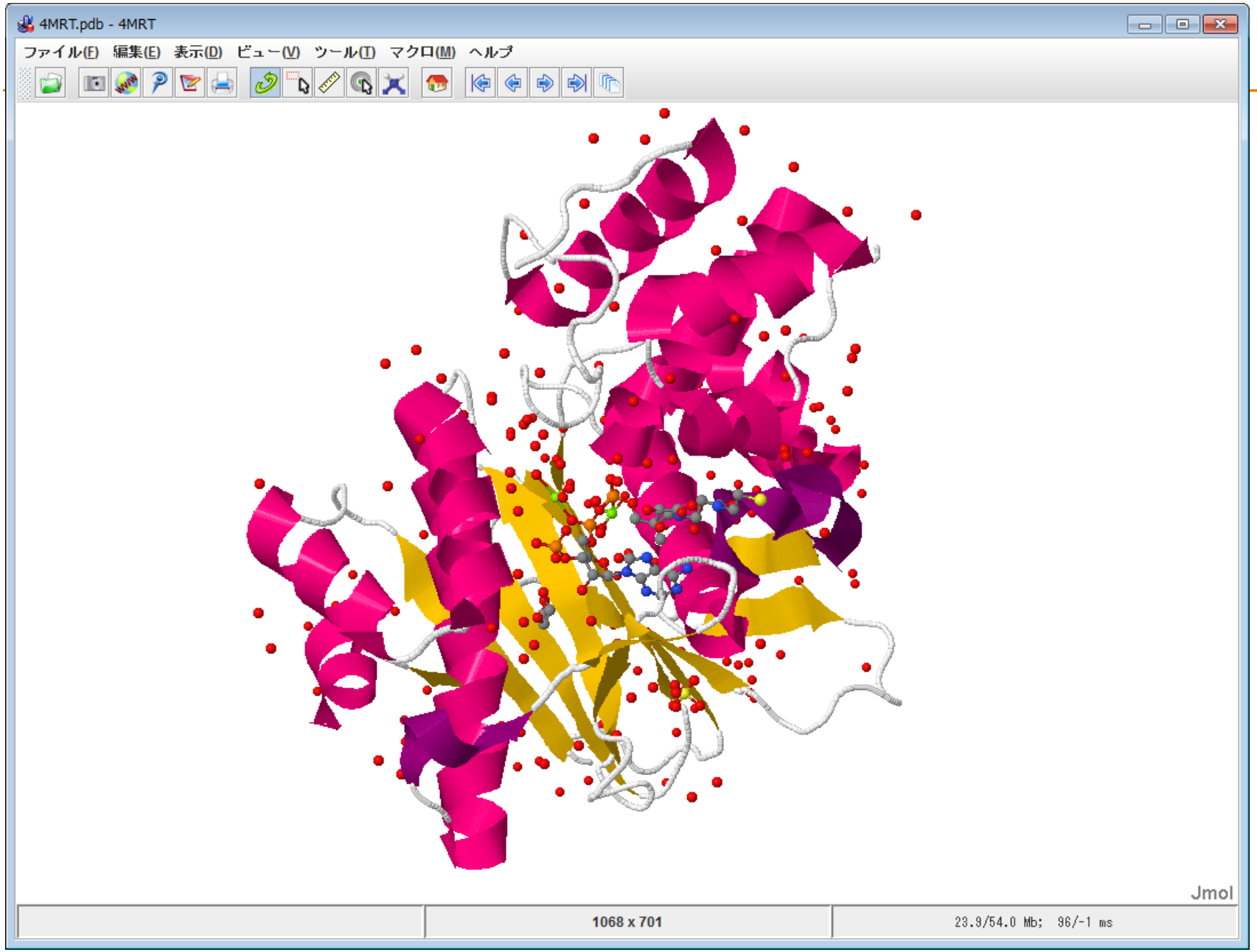
No symmetry
Stoichiometry: **Hetero 2-mer - AB**
Biological assembly 1 assigned by authors and generated by PISA (software)

Downloadable viewers:
Simple Viewer Protein Workshop
Kiosk Viewer

MyPDB Personal Annotations Hide

To save personal annotations, please **login** to your MyPDB account.

Deposition Summary Hide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ファイル(F) 編集(E) 表示(D) ビュー(V) ツール(T) マクロ(M) ヘルプ
Jmol
1068 x 701
23.9/54.0 Mb; 96/-1 ms

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ATOM      1  N   TYR C   8      28.289  16.437  30.736  1.00 30.26           N
ATOM      2  CA  TYR C   8      28.623  17.149  29.472  1.00 29.23           C
ATOM      3  C   TYR C   8      30.121  17.463  29.374  1.00 29.62           C
ATOM      4  O   TYR C   8      30.694  18.045  30.295  1.00 29.96           O
ATOM      5  CB  TYR C   8      27.790  18.437  29.351  1.00 28.95           C
ATOM      6  CG  TYR C   8      28.248  19.348  28.233  1.00 29.23           C
ATOM      7  CD1 TYR C   8      27.847  19.136  26.915  1.00 29.00           C
ATOM      8  CD2 TYR C   8      29.111  20.424  28.497  1.00 30.57           C
ATOM      9  CE1 TYR C   8      28.291  19.967  25.889  1.00 30.24           C
ATOM     10  CE2 TYR C   8      29.560  21.258  27.486  1.00 30.01           C
ATOM     11  CZ  TYR C   8      29.145  21.033  26.189  1.00 31.07           C
ATOM     12  OH  TYR C   8      29.610  21.851  25.195  1.00 31.72           O
ATOM     13  N   VAL C   9      30.735  17.114  28.246  1.00 26.60           N
ATOM     14  CA  VAL C   9      32.122  17.477  27.976  1.00 25.73           C
ATOM     15  C   VAL C   9      32.200  18.215  26.648  1.00 24.69           C
ATOM     16  O   VAL C   9      31.846  17.680  25.599  1.00 21.62           O
ATOM     17  CB  VAL C   9      33.069  16.235  27.966  1.00 25.06           C
ATOM     18  CG1 VAL C   9      34.519  16.656  27.787  1.00 25.50           C
ATOM     19  CG2 VAL C   9      32.888  15.419  29.239  1.00 24.57           C
ATOM     20  N   ALA C  10      32.689  19.456  26.685  1.00 24.40           N
ATOM     21  CA  ALA C  10      32.747  20.280  25.479  1.00 23.79           C
ATOM     22  C   ALA C  10      33.794  19.680  24.562  1.00 23.36           C
ATOM     23  O   ALA C  10      34.740  19.070  25.059  1.00 25.68           O
ATOM     24  CB  ALA C  10      33.113  21.721  25.829  1.00 23.10           C
ATOM     25  N   PRO C  11      33.627  19.830  23.231  1.00 22.26           N
ATOM     26  CA  PRO C  11      34.653  19.392  22.289  1.00 23.32           C
ATOM     27  C   PRO C  11      36.006  20.066  22.511  1.00 28.69           C
ATOM     28  O   PRO C  11      36.060  21.261  22.864  1.00 29.11           O
ATOM     29  CB  PRO C  11      34.085  19.784  20.931  1.00 22.13           C
ATOM     30  CG  PRO C  11      32.599  19.795  21.116  1.00 22.12           C
ATOM     31  CD  PRO C  11      32.331  20.071  22.568  1.00 21.91           C
ATOM     32  N   THR C  12      37.075  19.300  22.299  1.00 30.16           N
ATOM     33  CA  THR C  12      38.437  19.729  22.610  1.00 33.54           C
ATOM     34  C   THR C  12      39.331  19.881  21.373  1.00 33.71           C
ATOM     35  O   THR C  12      40.499  20.257  21.492  1.00 37.27           O
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ATOM     37  OG1 THR C  12      39.298  17.467  22.843  1.00 33.13           O
ATOM     38  CG2 THR C  12      38.255  18.464  24.781  1.00 34.27           C
ATOM     39  N   ASN C  13      38.804  19.571  20.195  1.00 34.37           N
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ATOM     42  O   ASN C  13      37.418  19.673  17.890  1.00 32.23           O
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Gaussianの使い方

Hydrogen.gif

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#N HF/6-311G**

comments

0 2
H
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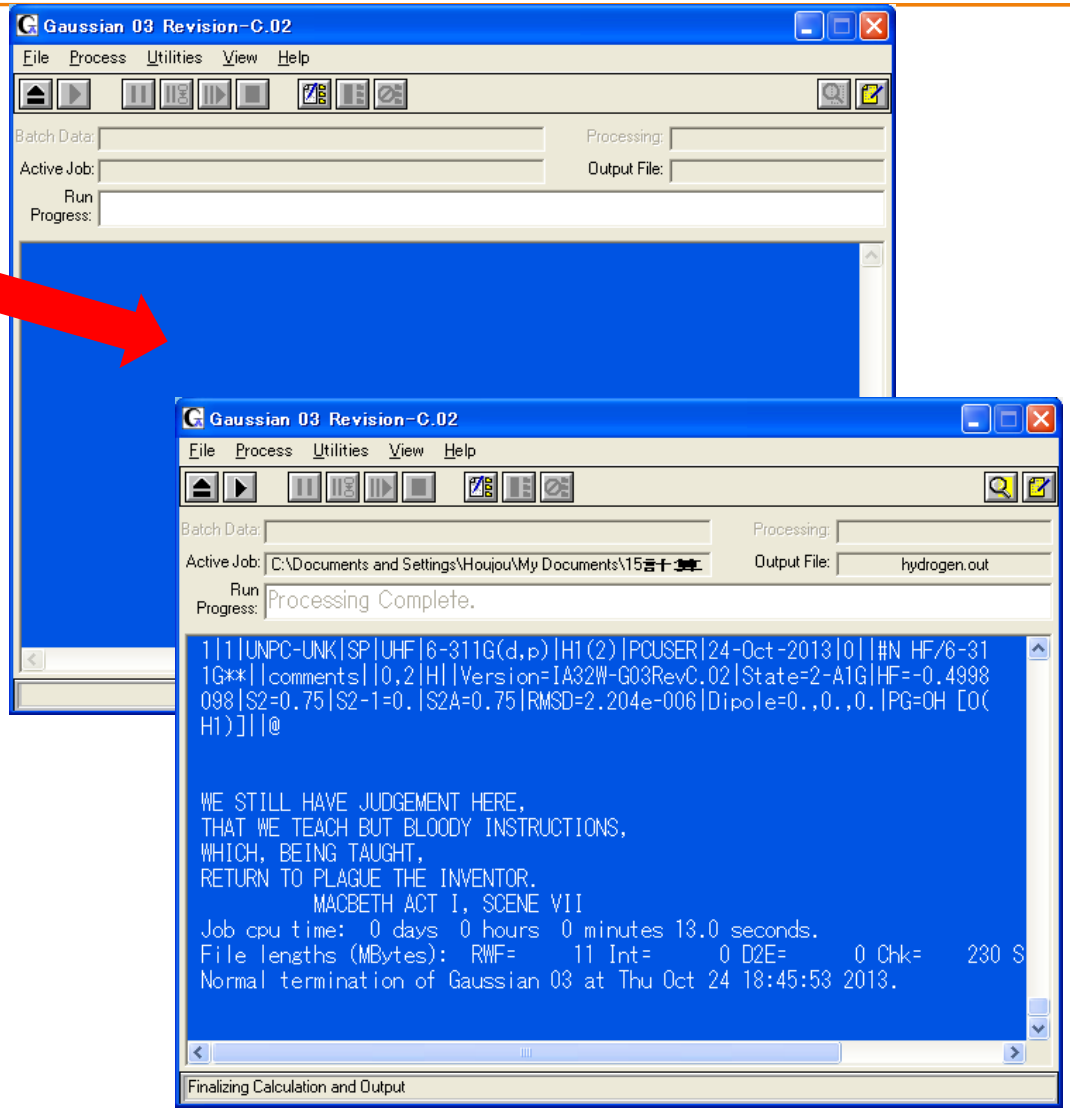

入力ファイル

%chk=default	チェックポイントファイルの指定
#N HF/6-311G**	出力フォーマット(Normal, Print, Terse) Hartree-Fock法,6-311G**基底関数
comments	コメント
0 2	電荷、スピン多重度
H	元素記号

分子構造の情報

XYZ座標で指定

```
water molecule

0 1
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
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内部参照座標（Zマトリクス）で指定

```
water molecule

0 1
O
H 1 r2
H 1 r3   2 a3

r2 1.0
r3 1.0
a3 104.5
```