----- Ver.9.9.1 -----   Dec. 25, 2005

(1) Molecular models of icosahedral higher fullerenes (C80, C180, C240, C320, C500, C540, C720, C960, C980, C1280) are newly assembled from scratch with Facio.

(2) GIAO isotropic shielding values calculated with Gaussian / WinGamess are read in and chemical shifts relative to the TMS absolute shielding value are shown in table.

----- Ver.9.8.9 -----   Nov. 29, 2005

(1) It was found again that there are cases where vibrational vectors of Gaussian normal mode calculation are not properly read.   This bug has been fixed.

----- Ver.9.8.8 -----   Nov. 28, 2005

(1) Resolution with which intensity and wave number of IR, Raman and VCD are saved as text file is changed from 5.0 (1/cm) in the previous version to 0.1 (1/cm).

(2) It was found that there are cases where vibrational vectors of Gaussian normal mode calculation are not properly read.   This bug has been fixed.

----- Ver.9.8.7 -----   Nov. 12, 2005

(1) The way to display a series of structure obtained by IRC calculation with Gaussian is modified.
   For example, if the calculation was performed for 13 points on IRC, results are stored in the formatted check file in the order of 7-6-5-4-3-2-1-8-9-10-11-12-13, in which the structure #7 corresponds to the transition state. The older version of Facio displays these structures in the order as stored, i.e. 7-6-5-4-3-2-1-8-9-10-11-12-13. Ver.9.8.7 displays them in the order of 1-2-3-4-5-6-7-8-9-10-11-12-13 so as to show continuous change of the structures.

(2) In IRC display mode, inter atomic distance, bond angle and dihedral angle are incorrectly measured. This bug has been fixed.

(3) Trajectory data obtained by ADMP or BOMD MD calculation with Gaussian can be visualized. Energy changes (nuclear kinetic energy, electron kinetic energy, potential energy and total energy) are plotted along the time in trajectory.

(4) Cartesian coordinate 1 and 2, and "free formatted XYZ" file are newly supported as an input file.
   Free formatted XYZ file is a simple XYZ file, in which each line consists of only atom symbol and x, y, z coordinates separated with at least one space. See the sample.xyz in the XYZ folder in Facio folder.

----- Ver.9.8.6 -----   Oct. 2, 2005

(1) Intensity and wave number of IR, Raman and VCD can be saved as text file.

(2) You can see atomic number with "Miscellaneous Menu >> Highlight Specified Atom"

----- Ver.9.8.5 -----   Sept. 24, 2005

(1) In a special case, CUBE MO data is incorrectly determined to be "truncated"
    with the warning message "CUBE data may be truncated", even if it is not so.
    This bug has been fixed.

----- Ver.9.8.4 -----   Sept. 17, 2005

(1) GUI for Gaussian ONIOM Layer specification has been implemented.

(2) VCD(Vibrational Circular Dichromism) spectrum is simulated.
    VCD calculations of *d*-Menthol and *l*-Menthol are included as example data.

(3) Displacement vectors of normal mode vibration are shown as arrows.

(4) You can use g03w.exe instead of g03.exe for command line execution of Gaussian.

----- Ver.9.8.3 -----   Aug. 27, 2005

(1) Completion of missing hydrogens has been implemented.

(2) Facio can read FORCE calculation data of MOPAC6,
    WinMOPAC3.0, 3.5, and 3.9 to show normal mode vibration as animation.

(3) You can capture the screenshot of main window of Facio and save as JPEG file.
    Unlike Windows' Alt-PrintScreen function, Facio's screenshot function excludes
    window frame and menu bar.

----- Ver.9.8.2 -----   Jul. 9, 2005

(1) For transition structure search using the STQN method, the reactant, product,
    and initial TS structure can be specified through GUI.

(2) Facio has failed to read PDB file which has MODEL and CONECT records.
    This bug has been fixed.

----- Ver.9.8.1 -----   Jun. 17, 2005

(1) SSH / SFTP client has been implemented. Through SSH / SFTP connection, Gaussian job can
    be submitted to batch job system on the remote server and calculation results can be retrieved
    form the server. Supported batch job systems are LoadLeveler and NQS.

----- Ver.9.7.6 -----   Apr. 18, 2005

(1) Facio and external programs can be installed in different disk drives each other.
    For example, Facio in D: drive and PC Gamess in C: drive.

(2) User-customized position and size of main window and position of Facio's worksheet
    is saved in Facio.ini.   See Edit menu >> Save Position and Size of Main Window

(3) Edit Tool Box :
    Selected Edit Menu items are separated from menu and packed in a box which can be
    placed anywhere in display. Edit Tool Box facilitates molecular modeling.
    See Miscellaneous menu >> Show Edit Tool Box

----- Ver.9.7.5 -----   Apr. 9, 2005

(1) Criteria to determine mesh representation of CUBE MO is now adjustable.
   If no mesh representation is shown, please increase Mesh Criteria value.

----- Ver.9.7.4 -----   Mar. 12, 2005

(1) IRC data (in Gaussian formatted check file) is visualized.

----- Ver.9.7.3 -----   Feb. 26, 2005

(1) Electrostatic Potential CUBE data calculated with PC GAMESS or Gaussian 03W
    is mapped onto Solvent Excluded Surface calculated with MSMS.
    The following graphics shows this feature.
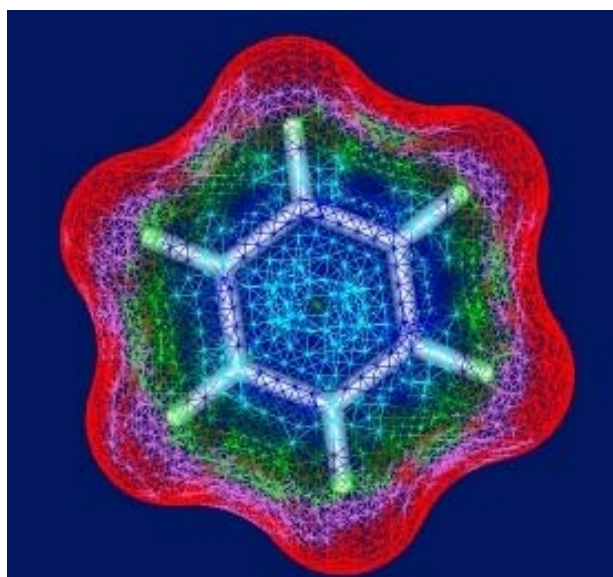
Electrostatic potential of Benzene mapped onto solvent excluded surface

(2) With Facio Ver.9.6.1 and Ver9.7.1, PC GAMESS input file for CUBE electrostatic potential and
   electron density has not been calculated even if user properly sets input options.
   This bug has been fixed.

(3) Utility which is useful for modeling of compound with symmetry are added.
   With this utility, atoms which are within ApproxityCriteria are exactly
   moved to Z axis. The parameter ApproxityCriteria is set in the Facio.ini.

----- Ver.9.7.2 -----   Feb. 5, 2005

(1) Visualization of Gaussian 03W CUBE molecular orbital and normal mode vibration
   has been implemented. Graphical Viewer of MO level and multiplicity is also built in.
   GUI for Gaussian 03W Utilities (CubeGen, FormChk, FreqCheck) are also created.

(2) Molekel is invoked within Facio.

(3) In the case that PC Gamess or WinGAMESS is placed in the folder whose absolute path
   contains "space", a required fonder (Facio) has not been properly produced. This bug
   has been fixed.

----- Ver.9.7.1 -----   Jan. 22, 2005

(1) GUI for MCSCF calculation has been implemented.
   Parameters in $DRT and $DET group are automatically set
   according to the charge and spin multiplicity.

(2) GUI for Gaussian 03W has been implemented.
   With this GUI you can make an input file (Gaussian job file, *.gjf) and
   start the execution of the job.
   Customized route section commands for individual user are stored in Facio.ini
   as CustomRoute1, CustomRoute2, ... and CustomRoute9.

   *** Visualization of Gaussian output, such as molecular orbitals and
   normal mode of vibration will be implemented in the next version of Facio. ***

(3) In the case of Gamess option $CONTRL NOSYM=0 and
   $DATA GROUP=(other than C1), Facio failed to read
   some orbital energies. This bug has been fixed.

(4) Symmetry of molecular orbital is displayed in the MO Viewer panel.

(5) In the cases other than GROUP=C1, molecular orbital numbers of HOMO and
   LUMO have not been properly calculated. This bug has been fixed.

(6) Utility which is useful for modeling of compound with symmetry are added.
   With this utility, atoms which are within ApproxityCriteria are exactly
   moved to XY plane or YZ plane. The parameter ApproxityCriteria is
   set in the Facio.ini.

(7) Winmostar is invoked within Facio.   http://winmostar.com/

(8) Examples of compounds with symmetry are included in the SymmetryUnique
   folder.

(9) In some cases, preferences has not been properly saved. This bug has been fixed.

----- Ver.9.6.2 -----   Nov. 14, 2004

(1) In the case of Gamess option $CONTRL NOSYM=0 RUNTYP=OPTIMIZE and
   $DATA GROUP=(other than C1), "COORDINATES OF SYMMETRY UNIQUE ATOMS"
   are output. But the output format is slightly different between
   PC GAMESS and WinGamess. And this diffecence causes an input error
   when WinGamess output is loaded. This bug has been fixed.

(2) New checkbox is added
   in the Menu>>Preferences>>External Programs.

   When coordinates of symmetry unique atoms are available,
   this checkbox determines whether only symmetry unique atoms are shown or not.
   This option is valid only for "Load New Gamess Output".

----- Ver.9.6.1 -----   Nov. 7, 2004

(1) Interactive pre/post-processor for WinGamess has been implemented.

    WinGamess is PC WIN32/GCC VERSION of GAMESS
      (VERSION = 19 MAY 2004 (R4))
    precompiled under the Cygwin environment by Nuno A.G. Bandeira.

        http://www.msg.ameslab.gov/GAMESS/dist.pc.html

    Facio makes an input file and execute WinGamess job
    with runscript.csh and ddikick.exe in the WinGamess package

(2) When CUBE MO data is loaded from punch file, MO energies are also
    loaded from the corresponding output file.
    There was no problem about this up to now. But it was found that
    MO energies are not properly loaded in special cases,
    for example,6-31G(d)/UHF calculation of ammonia cation radical. This bug has been fixed.

----- Ver.9.5.1 -----   Oct. 24, 2004

(1) Parameters in TINKER Key file is described as relative path name,
    when the absolute path name of TINKER parameter file contains "space",
    e.g. "C:\My Document\Tinker\params\amber.prm".

    In such a case, the author assumes that the TINKER is
    installed as follows.

            Tinker ------ bin ------ optimize.exe
                          |
                      --- params --- mm3.prm
                                        |
                                      -- amber.prm

        (folder name 'bin' may be other name)

                or

            Tinker ------ optimize.exe
                          |
                      --- params --- mm3.prm
                                        |
                                      -- amber.prm

        In both case, folder name 'params' is fixed.

    However, if the absolute path name of TINKER parameter file
    DOES NOT contain "space", parameters in TINKER Key file is described
    as absolute path name.

(2) Although alpha and beta orbitals are obtaied from UHF calculation,
    only alpha orbitals have been taken in the preveous version of Facio.
    Now Facio can display both orbitals of UHF calculation.
    For ICORBS input data of GAMESS, Facio can automatically set
    negative orbital numbers for beta orbital CUBE data and visualize them.

    For example,

HOMO and LUMO of H2O radical cation is #5 and #6 MO, respectively.
If you set GAMESS input option of ICORBS in UHF calculatio as follows

HOMO-2   and   LUMO+1,

$ELDENS in the GAMESS input file will be

$ELDENS IEDEN=1 ICORBS(1)=3, 4, 5, 6, 7,
-3, -4, -5, -6, -7 $END

where negative numbers are corresponding beta orbitals.

About this new feature, I appreciate the useful suggestion of
Prof. emeritus Ernst Schumacher (University of Bern), the author of
RUNpcg and Cygam which are the GUI for executing the GAMESS code.

http://www.chemsoft.ch/qc/RUNpcg.htm
http://www.msg.ameslab.gov/GAMESS/dist.pc.html

(3) Zoom In/Out operation can be performed with mouse wheel.

----- Ver.9.0.1 -----   Sept. 12, 2004

(1) Interface to Tinker-MM3 calculation has been implemented.
So you can perform geometry opitimization with Tinker-MM3.

Atom types which Facio can recognize are ...

1	C	sp3 Alkane
2	C	sp2 Alkene
3	C	sp2 Carbonyl
4	C	sp Alkyne
5	H	except on N, O, S
6	O	C-O-H, C-O-C, O-O
7	O	C=O Carbonyl
8	N	sp3
9	N	sp2 (Amide)
11	F	Fluoride
12	Cl	Chloride
13	Br	Bromide
14	I	Iodide
15	S	-S- Sulfide
16	S+	>S+ Sulfonium
17	S	>S=O Sulfoxide
18	S	>SO2 Sulfone
19	Si	Silane
21	H	-OH Alcohol
22	C	Cyclopropane
23	H	NH Amine/Imine
25	P	Phosphine
28	H	Amide
37	N	Pyridine
38	C	Cyclopropene

(but bond stretching parameter 38-38 is undefined in MM3)

39	N+	N sp3 Ammonium
40	N	N sp2 Pyrrole
41	O	O sp2 Furan
42	S	S sp2 Thiophene

```
44    H    SH Thiol
46    N    Nitro
47    O    Carboxylate
48    H    Ammonium
49    O    Epoxy
56    C    C sp3 Cyclobutane
57    C    C sp2 Cyclobutene
58    C    C=O Cyclobutanone
124   H    C-H Acetylene
```

----- Ver.8.7.1 -----   Jul. 30, 2004

(1) Mesh surface representation for MO, total electron density and
    electrostatic potential has been implemented.

----- Ver.8.5.1 -----   Jul. 5, 2004

(1) Using RUNTYP=RAMAN option, you can calculate Raman intensities
    with which Raman spectrum is simulated.

    About this new feature, I appreciate the useful suggestion of
    Prof. emeritus Ernst Schumacher (University of Bern), the author of RUNpcg.

(2) In order to demonstrate the modeling ability of Facio,
    highly complex molecular models for natural toxins listed below are
    included in the folder PDB/Toxins. Not only the final structures but also
    intermediate structures are included to show how I constructed them.

        Brevetoxin-A   Halichondrin-B
        Maitotoxin   Neosurugatoxin
        Okadaic Acid   Pinnatoxin-A

----- Ver.8.3.1 -----   Jun. 22, 2004

(1) Polynucleotide model is built from scratch
    with a help of Tinker 3.9 (nucleic.exe).

    Because of bugs in "nucleic.exe" module in Ver.4.1 and
    4.2 (before minor revision: Sept. 8, 2004),
    collision will occur between the complementary
    base pairs for B-form double helix (base pairs >= 4)
    and Z-form one.

    ****
    For B-form double helix, the bugs have been fixed
    in the Ver. 4.2 (minor revision: Sept. 8, 2004)
    ****

    However, the bugs on Z-form have not yet been fixed.

(2) It was revealed that external programs cannot be run in the root folder.
    Thus, Facio checks whether they are installed in the root folder or not
    before enabling the menu item for them.

----- Ver.8.0.2 -----   May 31, 2004

(1) The scale of IR spectrum is shifted in some cases other than
Japanese Windows system and Lorentzian line shape of IR spectrum is
incorrectly calculated. These bugs have been fixed.

About this bug fix, I appreciate the useful comment of
Prof. emeritus Ernst Schumacher (University of Bern), the author of RUNpcg,
which is a graphical interface for executing the GAMESS code.

http://www.chemsoft.ch/qc/RUNpcg.htm
http://www.msg.ameslab.gov/GAMESS/dist.pc.html

RUNpcg is a 'Dialect' GUI to be used in conjunction with Gamess.

'Dialect' is a general purpose programming language that includes
an integrated development environment with debugging support.

http://www.downlinx.com/proghtml/104/10441.htm

(2) Structure of an origosaccharide sample PDB (Raffinose.pdb)
was incorrect at the connection of fluctose and glucose.
Correct structure has been included in this version.

----- Ver.8.0.1 -----   Apr. 30, 2004

(1) Visualization of $CUBE/Molecular Orbitals which is the new feature of PC GAMESS 6.4.

(2) Bugs in deletion of isolated atom are fixed.

(2) Procedure AddHydrogen was modified.

----- Ver.7.5.1 -----   Apr. 5, 2004

(1) Glycosyl substituents are available for polysaccharide modeling.

(2) OH, Formyl, NH2 substituents are also available.

(3) Point group symmetry can be specified for GAMESS calculation.
Related parameters are GROUP and NAXIS.   (GROUP=C1, CN only)

(4) Array of Cartesian coordinates to freeze during
a geometry optimization will be set with a parameter IFREEZ.

(5) $STATPT METHOD=CONOPT   with a parameter IFOLOW

This can be used for locating transition states.

(6) When GAMESS calculation terminated abnormally, the reason will be shown.

(7) $VEC data (MO coefficients) can be retrieved from
GAMESS punch file and pasted to input file with GUESS=MOREAD.

(8) When molecular geometry is adjusted, the current value is also shown.

(9) Auto Centering is OFF by default. For proteins or nucleic acids, default is ON.

----- Ver.7.0.1 -----   Mar. 11, 2004

(1) Polypeptide model is built from scratch with a help of TINKER's protein.exe

    See the description of Tools Menu >> Polypeptide Builder.

(2) Interface to DFT calculation is implemented.
    DFT calculation is a new feature of PC GAMESS ver.6.4.

(3) Molecular geometry can be adjusted more precisely.
    For angle adjustment 0.1 degree is the minimum change and
    for distance 0.001 angstrom, if "Fine adjustment" is checked.

----- Ver.6.5.1 -----   Feb. 9, 2004

(1) IR spectrum can be simulated with IR intensities data,
    which is available in normal mode calculation.
    How to use : see the description of Tools Menu >> Normal Mode Vib. Viewer.

(2) Total electron density can be calculated with semiempirical MOs.

    GAMESS produces total electron density as CUBE data only when ab initio
    calculation is performed. But this feature makes it difficult to visualize
    the electron density of a very large molecule. Thus, the calculation of
    electron density using coefficients of semiempirical MO is implemented in
    Facio 6.5.1.
    How to use : see the description of Tools Menu >> Molecular Orbital Viewer.

(3) Bug fix in 'Delete Atom'.

    Fatal exception sometimes occurred when solitary atom was deleted.
    Solitary atom is an atom which has no bond to other atoms.

----- Ver.6.0.1 -----   Jan. 24, 2004

(1) $HESS group (Hessian Matrix) can be retrieved from GAMESS Punch
    and attached to the GAMESS input file using GAMESS option HESS=READ.

(2) The number of Imaginary frequency is checked
    after RUNTYP=HESSIAN calculation.

(3) IRC data (a series of structures obtained after RUNTYP=IRC calculation)
    is visualized.

(4) New GAMESS Input Options:

        $CONTRL   RUNTYP=SADPOINT
                            =IRC

        $STATPT   HESS   METHOD

        $BASIS   NDFUNC NFFUNC NPFUNC DIFFSP DIFFS

        $IRC   PACE SADDLE FORWRD NPOINT STRIDE

(5) If optimized geometry or saddle point is available, coordinates will be
  written in 15.10F format to the GAMESS input file for the next run.
  If not, it will be written in 8.3F format as in PDB file.

  Availability of the stationary point coordinates is shown
  in the GAMESS input option panel.

(6) You can select perspective projection or orthogonal projection.
  Orthogonal projection is useful especially when you adjust
  relative position and tilting angle of two separately loaded molecules.

  See also Utilities Menu > "Adjust Position and Tilting Angle".

----- Ver.5.0.1 -----   Dec. 24, 2003

(1) Isovalue surface of electron density and electrostatic potentials
  are displayed with dot surface representation.

(2) New GAMESS Input Options:

  MESH   Specifies desired density of points
              along each side of the cube.
              Values are COARSE, MEDIUM, and FINE.

  ELDENS   Electron density is calculated.
  ELPOT   Electrostatic potentials are calculated.

  MORB   MORB=0   (Generates Total Electron Density)
              MORB=xxx   (Generates Electron Density for MO # xxx)

(3) In the previous versions, Facio.ini was not read in
  on Windows XP.   This bug was fixed.

----- Ver.4.7.1 -----   Dec. 11, 2003

(1) OpenGL rendering has been fully revised.

  Result : For example, animation of normal mode vibration is displayed
              much faster than former versions.
              Compare Ver.4.6.1 and Ver.4.7.1.

(2) On Germany or French system, Facio has been freezed.
  This problem was fixed.

  Some European countries use a comma for a floating point separator
  instead of a period. In particular, StrToFloat function will
  cause an exception if the string passed to it has the wrong decimal
  separator.

(3) Exception (e.g. access violation) occurred during the excution
  of Facio is fully trapped. This feature can be customized by
  editing the following init record in Facio.ini.

    [AppControl]
    ExceptionMessage=ON

where
ON   ===> Trap exception
OFF ===> Egnore exception   (But Facio may be freezed in case of vital exception)

(4) Visualization of electron density and electrostatic potential is
not yet implemented in Ver.4.7.1.

----- Ver.4.6.1 -----   Nov. 7, 2003

(1) Facio can be launched as a command line application, which
accepts one command line argument (i.e. pdb file) at run time.

How to use :
MS-DOS prompt> Facio.exe xxx.pdb

where the xxx.pdb is a PDB file.

(2) Graphics rendering interval can be customized in Facio.ini file.
Since no GUI is provided for adjusting this parameter, please
edit the following init record in Facio.ini.

[Timer]
Interval=50

This means that graphics are rendered every 50 microseconds.
If your graphics card does not have sufficient power,
try to set this parameter higher value, e.g. Interval=100.
If your graphics card have sufficient power,
you can set it lower value, e.g. Interval=30. In that case,
Facio will more quickly respond to your mouse movement.
However, never set it 10 or lower : your machine may be freezed.

This feature is no more necessary for Ver.4.7.1 or higher

(3) MODEL records in PDB file are recognized.
Only one model is displayed and other models are omitted for clarity.

(4) Hydrogen atoms of standard residues in PDB file are
parsed to produce connectivity record.

(5) Hydrogen atom can be attached to lone atom.

----- Ver.4.5.1 -----   Oct. 17, 2003

(1) MO visualization is implemented for basis set MINI.
This means that MOs of all the atoms up to Rn can be
visualized. You can see 4f orbitals for lanthanides.

(2) New GAMESS input options(IREST and GUESS) are supported.
With input option IREST=-1, GAMESS execution can be
easily restarted where it left off.

(3) Several bugs about parsing Protein PDB files are fixed.