

ORBLOT 2.0: NBO Orbital Plotter

by

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I. INTRODUCTION

ORBLOT** is an interactive graphics package developed in conjunction with the Natural Bond Orbital (NBO) analysis of Weinhold and co-workers. The package has the following features:

- Creates *orbital diagrams*, displaying profiles of orbital amplitude along a selected vector passing through the molecule;
- Creates *contour diagrams*, displaying contours of orbital amplitude on a selected plane in the molecule;
- Creates *electron density diagrams*, displaying contours of total electron density on a selected plane in the molecule;
- Displays composite diagrams of one or more overlaid images on a Regis graphics device;
- Prepares files for printing images in HP LaserJet bitmap, TechSet bitmap, or PostScript format.

The hardware requirements for ORBLOT 2.0 are a VAX/VMS computer system, VT 240 graphics terminal, and either HP LaserJet or PostScript printer. The ORBLOT 2.0 program is distributed as a single Fortran source module. Most of the code is VAX FORTRAN and Fortran 77 compatible, but certain VMS-specific I/O calls and a Regis implementation of Calcomp PLOT10 graphics library commands are used to draw the graphics screen images on a VT 240-compatible device. Calcomp PLOT10 graphics libraries are provided for printing high-resolution graphics images on HP LaserJet or PostScript printers.

VMS-specific and device-specific driver libraries are grouped together for possible replacement by equivalent routines in other hardware environments (cf. the related Lahey Fortran GTEXT subroutine for IBM PC-compatible CGA/EGA/VGA graphics devices). However, no assurances are offered that the present software is usable with non-VMS systems.

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**The original ORBLOT was written by E. D. Glendening, J. E. Carpenter, and F. Weinhold (1985-1990). The program incorporates contouring routines written by D. P. Anderson (Chemistry Department Harris/7 System Manager; routines used and distributed with permission) and various HP and Regis graphics PLOT10-emulation routines written by John Carpenter, Mark Muyskens (Crim group) and Scott Ostrander (Weisshaar group) for the Chemistry Department system. Revisions incorporated in ORBLOT 2.0 were written by F. Weinhold (1992).

II. GETTING STARTED

Since the input for the ORBPLOT program is generated by the NBO program, you will first need to perform NBO analysis of the wavefunction for the molecule of interest. In particular, you should include the PLOT and FILE=JOBNAME keywords in the \$NBO keylist; see NBO Program Manual, Sections B.2.4, B.2.5.

The NBO program will automatically generate the files and default filenames assumed by ORBPLOT (e.g., C2H6.31, C2H6.32, ...) for jobname C2H6). With these input files, ORBPLOT can plot any desired natural localized orbitals, including natural atomic orbitals (NAOs), natural hybrid orbitals (NHOs), natural bond orbitals (NBOs), or natural localized molecular orbitals (NLMOs), as well as their respective "pre-orthogonal" counterparts (PNAO, PNHO, PNBO, PNLMO sets*). ORBPLOT can also display basis atomic orbitals (AOs) or canonical molecular orbitals (MOs) for the molecule of interest. Note that the basis labels and orbital numbering used by ORBPLOT conform to those of the NBO output.

Suppose, for example, that you have completed a Gaussian job called "C2H6" for ethane (with \$NBO PLOT FILE=C2H6 \$END keylist). Move to the directory containing output files C2H6.31, C2H6.32, ... , C2H6.42 and type RUN ORBPLOT to start the program.

ORBPLOT first asks for the jobname (type "C2H6") and displays the default filenames of the various required transformation matrices, as shown below:

```
-----
Files containing basis set info and transformation matrices

      AO      [C2H6.31]:
      PNAO    [C2H6.32]:
      NAO     [C2H6.33]:
      PNHO    [C2H6.34]:
      NHO     [C2H6.35]:
      PNBO    [C2H6.36]:
      NBO     [C2H6.37]:
      PNLMO   [C2H6.38]:
      NLMO    [C2H6.39]:
      MO      [C2H6.40]:
AO density matrix [C2H6.41]:
Basis label info  [C2H6.46]:

Are these entries OK ([Y]/N)?
-----
```

Throughout the program, simply press <CR> (carriage return) to accept any displayed [default] option enclosed in brackets.

Type the new filename if you have altered a default NBO filename, or "N" if a file is unavailable;

*The pre-orthogonal orbitals (lacking only the final interatomic orthogonalization step) resemble the idealized "textbook" free-atom shapes, and their overlaps qualitatively suggest the strength of orbital interactions.

otherwise, press <CR> to accept the displayed filenames. You must always provide the AO basis info (.31 file), as well as the transformation matrices for any basis set you wish to select with the BASIS command (see Section III). The AO density matrix (.41 file) is needed only if you wish to plot the electron density. Note that the .41 file refers to the AO matrix representation of the density operator, and thus differs from the Fock-Dirac density matrix (for non-orthogonal basis AOs) by a similarity transformation.

After this initial program setup, the ORBPLOT "Command:" prompt should appear, and you're ready to begin computing and viewing orbital, contour, and electron density diagrams. In the next Section, we list the commands which make this possible.

III. ORBPLOT INSTRUCTIONS

ORBPLOT is controlled by the entering program instructions in response to the ORBPLOT 'Command:' prompt. ORBPLOT is case-insensitive, free-format, and only the first unique letters of an instruction are required to invoke the instruction. Some instructions require additional information, and often ORBPLOT obtains this information by asking questions. However, several instructions require that one or several parameters be specified on the 'Command:' line. More information about this is presented below, or in the on-line HELP utility for each command. Note that the display bar at the top of the screen lists the possible ORBPLOT commands, while the display bar along the right edge of the screen summarizes current settings and memory storage, and will be updated each time you execute a command.

ORBPLOT has essentially four types of instructions:

- (1) *Compute Instructions* (CONTOUR, ORBITAL, DENSITY) compute the orbital amplitudes or electron density at a set of grid points, fit the amplitudes, generate the vectors of a graphical image, and store the vectors in memory. Each compute instruction also calls appropriate view instructions to draw the image on the graphics screen. The information bar along the right edge of the command screen summarizes the stored information for the eight most recent compute instructions.
- (2) *View Instructions* (SHOW, DRAW) retrieve one or more stored images from memory and send them to the desired display device (directly to the screen, or as an output file to the disk for subsequent printing on a laser printer). These instructions allow multiple images to be overlaid in a single frame.
- (3) *Select Instructions* (BASIS, PLANE, VECTOR, SIGN, LINES) select the current coordinate system and other attributes of the graphical images being computed. Current selections are summarized along the right edge of the command screen.
- (4) *Information Instructions* (LABEL, STORAGE, HELP) provide information on current storage assignments and available orbital selections. In addition, an extensive on-line HELP utility describes the syntax, parameters, and function of each command (e.g., type HELP SHOW for information about the SHOW command).

The EXIT command terminates program execution.

Below, we briefly describe each ORBPLOT instruction (the first unique letters of each instruction are capitalized):

Instruction	Arguments	Description
<i>Compute Instructions</i>		
Orbital	I	Requests that an orbital diagram of a selected orbital (<i>I</i> in the current basis set, see the BASIS instruction) be computed along the current vector (see the VECTOR instruction). This instruction should always be followed by an orbital number. For example, ORBITAL 24 requests that the diagram for the 24th orbital be drawn. (The orbital numbering is identical to that of the NBO output.)
Contour	I	Requests that a contour diagram of an orbital (<i>I</i> in the current basis) be computed on the current plane (see the PLANE instruction). For example, CONTOUR 2 will compute the contour diagram of the 2nd orbital (orbital numbering identical to that of the NBO output).
DEnsity		Requests that the total molecular electron density be computed on the current contour plane. This command requires that the density matrix be available, and that the current basis set (see the BASIS instruction) be orthogonal. Contours of electron density are in units of electrons per cubic angstrom.
<i>View Instructions</i>		
SHow	I J...	Instructs ORBPLOT to draw (on the screen) the orbital, contour, or electron density diagram that is stored in a specified memory location (see discussion of graphical image storage and the STORAGE instruction). For example, SHOW 4 draws the diagram stored in memory location 4. SHOW can also be used to overlay several diagrams. Thus, SHOW 2 5 displays the diagrams stored in memory locations 2 and 5.
DRaw	I J...	Similar to instruction SHOW, but causes ORBPLOT to write an image file to the disk for later printing with a LaserJet or PostScript-compatible printer. The ORBPLOT image file may be specified to be in HP-PCL bitmat format (e.g., named C2H6.HPO), TechSet bitmap format (e.g., named C2H6.TSO), or PostScript format (e.g., named C2H6.PSO).
<i>Select Instructions</i>		
Basis	<i>type</i>	Permits the user to select the basis set used for the orbital, contour, and electron density diagrams. For example, the command BASIS NBO selects the NBO basis, and all subsequent diagrams will be for the NBO basis (until the BASIS command is used again). The initial default is the AO basis. For open-shell systems, the commands "BASIS a" or "BASIS b" select (a)lpha or (b)eta spin set for current basis (if applicable).

Instruction	Arguments	Description
Plane		Allows the user to specify the plane to search when computing contour and electron density diagrams. If a plane has not been previously specified when the user requests a contour or electron density diagram, this command is invoked automatically. See more about this command below. The initial default is the plane containing the first three atoms of the molecule, with the coordinate origin midway between the first two atoms.
Vector		Allows the user to select the vector to be searched when computing orbital diagrams. If a vector has not been previously specified when the user requests an orbital diagram, this command is automatically invoked. See more about this command below. The initial default is along a line containing the first two atoms, with coordinate origin midway between these atoms.
Lines		Allows the user to specify the first contour, the contour step size, and the number of contours drawn. This instruction also lets you adjust the lengths and spacing of the dashed lines. Initial defaults are provided for all parameters. The default outermost contour (0.03162 a.u.) corresponds roughly to the empirical van der Waals radius [see Bader and coworkers, <i>J. Chem. Phys.</i> 46 , 3341 (1967)].
Sign		Changes the sign (phase) of orbitals that are computed by ORBITAL and CONTOUR commands. Note that SIGN has no effect on diagrams already stored in memory.

Information Instructions

Storage		Provides summary information about the diagrams currently stored in memory. See discussion of graphical image storage below. A summary of current storage is also displayed in the bar along the right edge of the command screen.
Label		Displays a list of orbital labels for the current basis set. The numbers and labels correspond to those used in the NBO output.
Help	<i>command</i>	Provides a brief summary of command syntax, parameters, abbreviation, and function for each command. For example, the command HELP DRAW (or H DR) displays information about the DRAW command.

other

Exit		Normal exit from the ORBPLOT program.
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Note: As noted above, *default* answers are generally provided, always in brackets. Defaults can be selected by simply hitting <CR> in response to the question.

IV. DEFINING A PLANE OR VECTOR

Before computing a contour or electron density diagram, a plane must be specified. The following is sample input:

```

-----
                        Definition of Plane

Enter three atom numbers      [  1,  2,  3]: 3 1 4
Enter fraction to locate origin [          0.5]:
Enter two rotation angles     [  0.0,  0.0]:
Enter shift of plane along normal [          0.0]:
Enter minimum and maximum X values [ -3.0,  3.0]:
Enter minimum and maximum Y values [ -3.0,  3.0]:
Enter number of steps NX and NY  [   25,   25]:

Are these values OK ([Y]/N)?
-----

```

The following algorithm is used to determine the plane:

- (a) [Enter three atom numbers] AXIS 1 coincides with the line of nuclear centers between the first and second atoms, directed from the first toward the second. AXIS 2 is orthogonal to AXIS 1 in the plane that contains all three atoms, directed from AXIS 1 toward the third atom. Note that the atom numbering is the same as that used by the NBO analysis (and in the AOINFO file). Pad the entry with zeros when examining single atoms or diatomics.
- (b) [Enter fraction to locate origin] 0.0 places the origin on the first atom, and 1.0 places the origin on the second. Other values locate the origin accordingly. AXIS 1 and AXIS 2 intersect at the origin.
- (c) [Enter two rotation angles] First, AXIS 2 is rotated about AXIS 1 by the first rotation angle (in degrees). Second, AXIS 1 is rotated about AXIS 2 by the second rotation angle (in degrees).
- (d) [Enter shift along normal] The plane defined by AXIS 1 and AXIS 2 is shifted by a specified number of angstroms toward the viewer.

This completes the selection of a plane. The X (horizontal) axis coincides with AXIS 1, and the Y (vertical) axis with AXIS 2. Note that by suitable choices of these seven input parameters you can specify *any possible* choice of the contour plane. Usually, the plane will be chosen to pass through three atoms, and in this case the final three parameters (two rotation angles and normal shift; default zero) can be ignored. However, by setting either of the rotation angles to 90° one can view contours in the plane of pi-bonding with respect to the corresponding pair of atoms, and by setting a non-zero normal shift one can select cross-sections through a pi bond above or below the nodal plane. Thus, these seven parameters usually make it convenient to orient the contour plane with respect to significant chemical features.

The answers to the remaining three questions [X range (in angstroms), Y range, number of X and Y steps] are used to select a window (and set of grid points) on this plane. A 25x25 grid is generally sufficient for contour diagrams of first-row compounds. However, one may wish to enhance the resolution (say, to 50x50), particularly when the image has extensive nodal character.

The selection of a vector for orbital diagrams is similar.

```

-----
                        Definition of Vector
Enter two atom numbers      [   1,   2]:4 7
Enter fraction to locate origin [   0.5]:
Enter minimum and maximum X values [-2.0, 2.0]:-3 3
Enter min and max function values [-1.0, 1.0]:
Enter number of steps NX    [   100]:

Are these values OK ([Y]/N)?
-----

```

The vector coincides with the line of nuclear centers between the two atoms specified, directed from the first atom toward the second. The fraction 0.0 places the origin on the first atom, while a fraction of 1.0 places the origin at atom two.

V. GRAPHICAL IMAGE STORAGE

ORB PLOT is currently configured with eight (PARAMETER MAXSTR) memory locations, each location capable of storing one graphical image. Each time the ORBITAL, CONTOUR, or DENSITY instruction is used, the image computed is stored in one of these memory locations, the first image in location 1, the second in location 2, and so on. Once all eight memory locations are filled, ORB PLOT begins writing new images over the old ones. Thus, the ninth image is written to location 1, the tenth to location 2, etc. The most recent entry written in the memory array is marked by an asterisk (*) in the "current settings" display area at the right edge of the screen.

The user can also monitor the contents of the memory locations with the STORAGE instruction. The following is a sample of the output written in response to this instruction:

```

-----
Loc.  Type  +/-  Orbital  Projection (atoms)
-----
  1    CONT  +    AO   12    PLANE  1 (1 2 3)
  2    CONT  +    PNLMO 5a   PLANE  2 (12 5 8)
  3    CONT  -    PNLMO 5b   PLANE  2 (12 5 8)
  4    ORB   +    NAO   14    VECTOR 1 (1 2)
  5    DEN
->6    CONT  +    PNBO 23a  PLANE  2 (12 5 8)
-----

```

As seen in this example, the STORAGE instruction provides information about the type of diagram (Orbital, Contour, Density), phase (+/-), basis type, orbital number, spin (a/b, if applicable), and projection subspace (Plane or Vector, with reference atom numbers) for each image currently stored in memory. This supplements the "current settings" information on the command screen, and is particularly useful if you make frequent changes of projection plane, orbital phases, etc. Note that the pointer (->) marks the memory location of the most recent stored image.

VI. GRAPHICAL INTERFACE TO ORBPLOT

ORBPLOT uses two primitive (pen draw, pen move) PLOT10 graphics commands. PLOT10 emulation routines for VT240 Regis graphics, HP-PCL LaserJet graphics, TechSet bitmap graphics, and PostScript output are provided with this distribution. Interfacing ORBPLOT to other graphics drivers should be relatively simple.

ORBPLOT calls the following PLOT10 routines (for screen display):

- SR PLOTS(HEIGHT,WIDTH,OUTLINE)

This routine initializes the graphics screen, preparing a window of dimension HEIGHT x WIDTH (REAL*4, in cm). An outline is added if OUTLINE (REAL*4) is set to 1.0.

- SR PLOT(X,Y,IPEN)

This routine performs either a pen move (IPEN=3) or a pen draw (IPEN=2) to the point X,Y (REAL*4, in cm) within the window specified in SR PLOTS.

PLOT10 routines are included in this distribution for writing HP bitmaps (SR HPLOTS, SR HPLOT), TechSet bitmaps (SR TPLOTS, SR TPLOT), and PostScript output (SR PSPLOTS, SR PSPLOT). The HP orbital bitmap (e.g., C2H6_5.HPO) can be printed with a command of the form

```
PRINT/PASSALL/QUEUE=HPLJQ C2H6_5.HPO
```

after you exit the ORBPLOT program ("HPLJQ" stands for the LaserJet queue on your installation). Similarly, the PostScript file (e.g., C2H6_5.PSO) can be printed with the command

```
PRINT/QUEUE=LN03$POST C2H6_6.PSO
```

where "LN03\$POST" identifies a PostScript printer. To print the TechSet orbital bitmap (say, C2H6_5.TSO), you must have the TechSet formatter program [PC version: ACS Software, 1155 Sixteenth Street, NW, Washington, DC 20036, (202) 872-4564]. If the file is assigned to Fortran logical file number 25 (say), you can include "#25" in any TechSet graphics (.GR) command. For example, if file PRINTIT.DAT contains the lines:

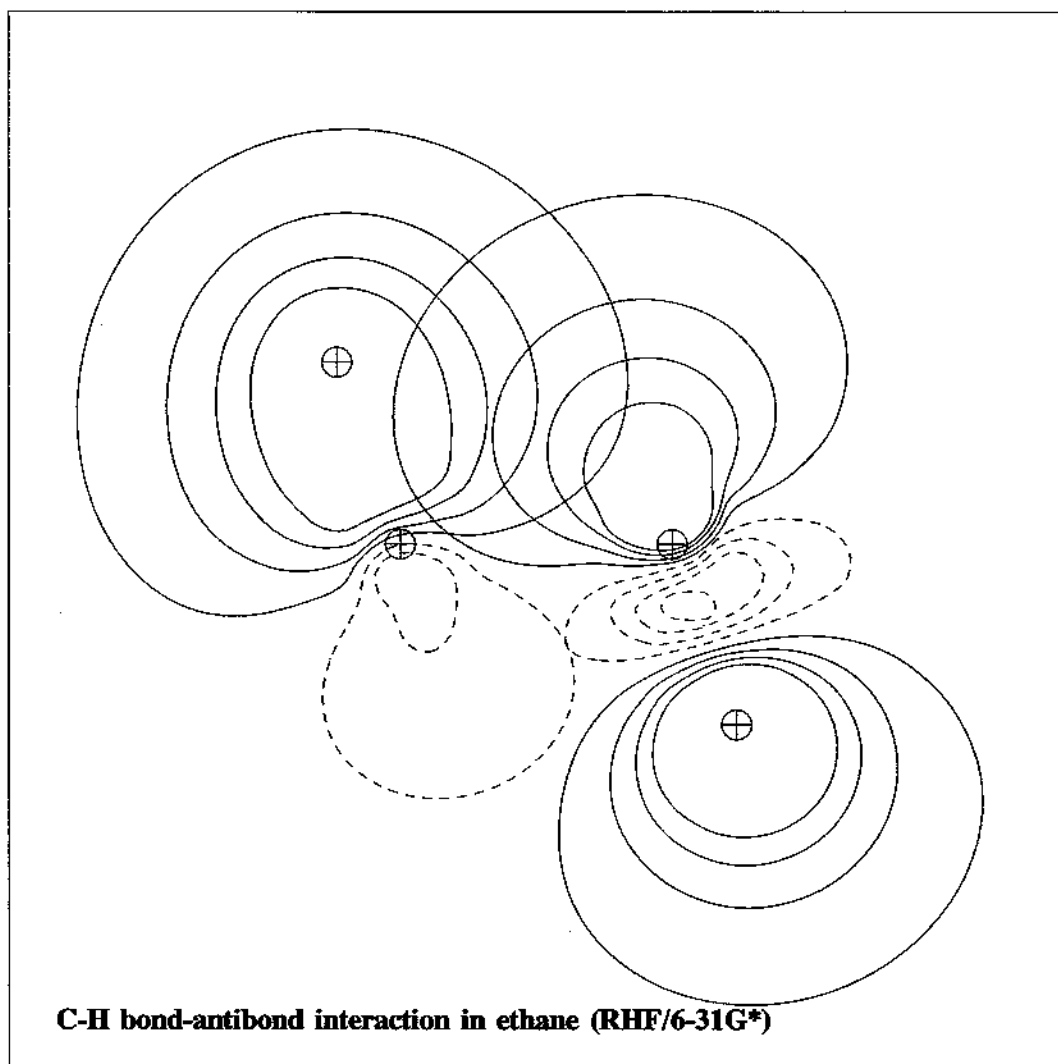
```
.GR<<#25>>
```

```
#BC-H bond-antibond interaction in ethane (RHF/6-31G*)#N
```

the command

```
TECHSET PRINTIT.DAT
```

will draw the bitmap with an accompanying caption as illustrated below:



Note that TechSet bitmap files are generally smaller than corresponding HP bitmap files, and they produce identical output on the HP LaserJet printer. PostScript and TechSet files contain only printable ASCII characters (rather than escape codes), and are therefore more suitable for editing, combining with other text or graphics material, E-mail transmission, and so forth.

To report errors, make suggestions, etc., please send E-mail comments to WEINHOLD (@CHEM.WISC.EDU) or call (608) 262-0263.