

Plot Input Files for Ternary and Binary Plots

DDBSP – Dortmund Data Bank Software Package



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Introduction

The program `DDBMDI PLOT` is a plot program which reads its commands from text files. These text files have the extensions “.D2P” for 2D-x,y plots and “.DTP” for triangle plots.

This paper describes both formats.

The D2P-x,y Format

List of Keywords

Keyword	Description
DEVICE	Obsolete and ignored. In old DOS time this numeric value (0-ask, 1-Terminal, etc.) was used to determine the output device. These old output devices are not supported anymore.
TITFNT	Font number for the title lines. The number ranges from 1 to 6 and relates to a font list with six font types.
TITDEF	This tag is followed by three numbers: <ol style="list-style-type: none"> 1. Line Number If the number is positive, the title is displayed above the drawing rectangle. Line no. 1 is the bottom line; higher numbers will show the title line above the bottom line. If the number is negative, the title is displayed at the right side of the drawing box and is flushed left. Larger negative numbers denote that the line is drawn at a lower position. 2. Center Code 1 for flush left, 2 for centered, 3 for flush right related to drawing rectangle, -1 left justified to display, -2 centered to display, -3 right justified to display. This code is ignored if line numbers are negative. 3. Color number The number range is from 1 to 16 and relates to a color list with 16 changeable entries.
TITLE	This tag is followed by a text. Leading blanks are ignored. If leading blanks are needed, use the ampersand. Blanks following an ampersand are drawn. Example: TITLE & Text with four leading blanks The line might contain special characters for indices ~ ⇒ up ^ ⇒ down CtrlG ⇒ mathematical character for the following character (CtrlG is character no. 7) CtrlP# ⇒ marker symbol (#=0..9, CtrlP is character no. 16)
FNTSIZ	Size of font as a floating point value. Normal sized fonts have a value of 0.25. Larger values denote larger fonts.
PNTSIZ	Size of points and markers inside the drawing rectangle. Normal (preset) value is 0.25.
FRAME	This tag is followed by four floating point values ranging from 0. to 1.

1. Left border of the drawing rectangle
2. Bottom border
3. Width
4. Height

The values are scaled. That means with a drawing area of 100 times 100 pixels the line
 FRAME 0.1 0.2 0.75 0.5
 indicates that the left border is at 10 pixels (0 . 1), the bottom line is at 20 pixels (0 . 2),
 the right line is at 85 pixels (0 . 1+0 . 75) and the top line is at 70 pixels (0 . 2+0 . 5).
 These values are relative values because the drawing is scaling by increasing or
 decreasing the size of the window.

XLABEL	Abscissa label
YLABEL	Ordinate label
XSCALE	This tag is followed by three floating points values: <ol style="list-style-type: none"> 1. Minimum value 2. Maximum value 3. Step width If this tag is missing the plot is scaled to its limits so that everything is visible.
YSCALE	Equivalent to XSCALE
XFORM	Output format of numbers on the abscissa label. FORTRAN format statement are used (like F10 . 2) for some historical reasons.
YFORM	Equivalent to XFORM
SCLTIC	Type of scale ticks <ol style="list-style-type: none"> 1 ⇒ Ticks at the bottom and left line of the drawing rectangle. Larger ticks for main values and one smaller tick between major ticks. 2 ⇒ Ticks at the bottom and left line of the drawing rectangle. No intermediate smaller ticks. 3 ⇒ Ticks at all four line and additional minor ticks 4 ⇒ Ticks at all four line but no additional minor ticks 10 ⇒ Lines all through the drawing rectangle Negative numbers from -1 to -4 denote that the ticks are drawn outside the drawing rectangle.
SCLFNT	Font number of the x- and y-axis labels (number from 1 to 6)
SCLVAL	Not supported any more
NULLIN	A line all through the drawing frame is drawn for y=0 if the value behind NULLIN is 1.
DATLBL	This line can be used to give a following DATAXY line or point list a special label which is used only for further information.
DATDEF	This tag is followed by three integer values <ol style="list-style-type: none"> 1. Number of points in the next DATAXY block If the number is negative the DATAXY doesn't contain the values themselves but a filename where the data are given in x- and y-columns. 2. Line or marker type -1 denotes a line, positive numbers from 1 to 50 with several duplicates denote marker types. 3. Color index

The index range is from 1 to 16.

DATFRM	Format of the numbers in the DATAXY block. FORTRAN format statements are used. Example: DATFRM F10.2,5X,G10.3
DATXCV	Conversion rule for x values. Possible operators are given with an example: <ul style="list-style-type: none"> • *760. ⇒ x=x*760. • LN ; -5. ⇒ x=log(x)-5. • /2. ; SQR ⇒ x=sqrt(x/2.) • LOG ⇒ x=log10(x) • 1/X ; EXP ⇒ x=exp(1./x) <p>The semicolon is used as a separator between operators. The evaluation sequence is from left to right.</p>
DATYCV	Equivalent to DATXCV for y values.
DATAXY	In the lines behind this tag the list of x- and y-values follows. The format of the lines is given behind the DATFRM tag and the number of points is given behind the DATDEF tag. It is possible to write a \$ sign followed by a number at the end of a line. This is used for data point identification in RecVal.
EXTERN	This tag is followed by a filename. This file can contain another D2P file or a DXP file with plot extensions. The DXP format is described later.
NEW	A D2P file can contain multiple plots. This tag separates these plots.
PROJCT	This tag denotes a RecVal project from which this plot has been created.

Example

```

EXTERN D:\SCRATCH\PLOT13.DXP
TITFNT      3
TITDEF 1 1 1
TITLE      H^2~O
TITDEF 2 1 1
TITLE      Butane
FRAME      0.1200  0.1000  0.7500  0.7500
XLABEL     x^1~
YLABEL     h~E^/J mol~-1^
SCLFNT     3
PROJCT     D:\SCRATCH\TMP0005.rvp
FNTSIZ     0.2500
pntSIZ     0.2500
NULLIN     0
DATFRM     (2F12.0)
DATFRM     (2g12.5)
DATDEF     22 13 2
DATLBL     35 HE 00235 ref2213 FRIESE T.,THESIS UNIV. DORTMUND(1998).
DATAXY
 0.25000E-01 -288.50          $ 86
 0.50000E-01 -534.30          $ 87
 0.75000E-01 -723.90          $ 88
 0.10000      -854.90          $ 89
 0.15000      -958.50          $ 91
 0.17500      -958.20          $ 92
 0.20000      -938.50          $ 93
 0.22500      -910.70          $ 94
 0.25000      -879.30          $ 95
 0.27500      -845.20          $ 96
 0.30000      -806.80          $ 97
 0.36000      -717.20          $ 98
 0.42000      -635.70          $ 99
 0.48000      -559.80          $ 100
 0.54000      -490.50          $ 101
 0.60000      -430.20          $ 102
 0.66000      -381.30          $ 103
 0.72000      -335.40          $ 104
 0.78000      -291.60          $ 105
 0.84000      -242.70          $ 106
 0.90100      -178.20          $ 107
 0.95900      -86.000         $ 108
    
```

The DTP-x,y,z Format

List of Keywords

Keyword	Description
DEVICE	Obsolete and ignored. In old DOS time this numeric value (0-ask, 1-Terminal, etc.) was used to determine the output device. These old output devices are not supported anymore.
TITFNT	Font number for the title lines. The number ranges from 1 to 6 and relates to an font list with six font types.
TITDEF	This tag is followed by three numbers: <ol style="list-style-type: none"> Line Number If the number is positive the title is displayed above the drawing rectangle. Line no. 1 is the bottom line; higher numbers will show the title the bottom line. If the number is negative, the title is displayed at the right side of the drawing

- box and are all flushed left. Larger negative numbers denote that the line is drawn at a lower position.
- 2. Center Code
1 for flush left, 2 for centered, 3 for flush right related to drawing rectangle, -1 left justified to display, -2 centered to display, -3 right justified to display. This code ignored if line numbers are negative.
- 3. Color number
The number range is from 1 to 16 and relates to a color list with 16 changeable entries.

TITLE	This tag is followed by a text. Leading blanks are ignored. If leading blanks are needed, use the ampersand. Blanks following an ampersand are drawn. Example: TITLE & Text with four leading blanks The line might contain special characters for indices ~ ⇒ up ^ ⇒ down CtrlG ⇒ mathematical character for the following character (CtrlG is character no. 7) CtrlP# ⇒ marker symbol (#=0.9, CtrlP is character no. 16)
FRAMET	This tag is followed by three floating point values ranging from 0. to 1. 1. Left border of the triangle 2. Bottom border of the triangle 3. Width of the triangle (always equilateral) The values are scaled. That means with a drawing area of 100 times 100 pixels the line FRAMET 0.1 0.2 0.75 indicates that the lower left edge is at x=10 pixels (0.1) and y=20 pixels (0.2), the right edge is at x=85 pixels (0.1+0.75) and the top edge is at y=70 pixels (0.2+0.5). These values are relative values because the drawing is scaling by increasing or decreasing the size of the window.
LLABEL	Label of the left edge
ULABEL	Label of the upper edge
RLABEL	Label of the right edge
FNTSIZ	Size of points and markers inside the drawing rectangle. Normal (preset) value is 0.25.
SCLTIC	This tag contains integer number defining the types of ticks or lines shown inside the triangle. If the number is negative, short ticks are drawn at 10 mole percent positions. If the number is positive lines are drawn at 100 /code positions. Example: SCLTIC 10 ⇒ 9 lines at 10, 20, 30, etc. mole percent SCLTIC 5 ⇒ 4 lines at 20, 40, etc. mole percent
SCLFNT	Font number of the x- and y-axis labels (number from 1 to 6)
DATFIL	This tag denotes a file with data columns
DATTYP	This tag is followed by a five digits number: nppcc n ⇒ number of phases (1 or 2) p ⇒ phase (1: liquid 2: vapor)

c ⇒ components given (2 component digits: 12 ⇒ Component 1 and 2 present)

DATDEF	This tag is followed by five numbers. <ul style="list-style-type: none"> • Number of points following in the DATAXY block • Color index • Line (0 ⇒ tie line is invisible, other values ⇒ tie line is shown) • Marker type for the composition in phase 1 • Marker type for the composition in phase 2 • Number n. Only every nth line is displayed. If n=1 every line is shown, if n=5 only every fifth line is drawn.
<hr/>	
DATFRM	Format of the columns in the DATAXY area. FORTRAN format statements are used.
<hr/>	
DATXCV	Conversion rule for compositions (see description of operator in D2P description).
<hr/>	
DATAXY	After this tag the lines with the compositions follow. <ol style="list-style-type: none"> 1. Mole fraction of component 1 in phase 1 2. Mole fraction of component 1 in phase 2 3. Mole fraction of component 2 in phase 1 4. Mole fraction of component 2 in phase 2
<hr/>	
EXTERN	This tag is followed by a filename. This file can contain another D2P file or a DXP file with plot extensions. The DXP format is described later.
<hr/>	
NEW	A DTP file can contain multiple plots. This tag separates these plots.

Example

```

EXTERN D:\SCRATCH\PLOT.DXP
FNTSIZ 0.2500
TITFNT 2
SCLFNT 2
SCLTIC -5
FRAMET 0.1300 0.1500 0.6500
LLABEL &(1)
ULABEL &(2)
RLABEL &(3)
; LLE data
DATFRM(4f10.0)
DATTP 21112
DATDEF 5 3 1 6 6 1
DATAXY
0.83400 0.15600 0.03500 0.05500
0.64500 0.31900 0.03700 0.09900
0.53400 0.40400 0.05400 0.16400
0.39200 0.48600 0.07300 0.21000
0.27900 0.49800 0.09800 0.28300
; LLE data
DATFRM(4f10.0)
DATTP 21112
DATDEF 4 2 -1 0 0 5
DATAXY
0.99920 0.00000 0.02638 0.00000
0.97500 0.02381 0.02793 0.00846
0.95500 0.04340 0.02913 0.01499
0.93500 0.06289 0.03027 0.02119
    
```

The DXP Plot Extension File Format

The DXP files are normally included in D2P and DTP file via the EXTERN command. These file contains some additional text and graphical elements for decoration purposes.

List of Keywords

Keywords	Description
LIMIT	Set scale of drawing (number of pixels in the current drawing window). Four numbers have to be given: Left, Right, Bottom, Top Example: LIMIT 0 300 0 300 A position of x=10,y=10 would be in lower left corner, a value of x=290,y=290 would be in the upper right corner
LINE	This tag can be followed by x,y pairs. It draws lines.
BOX	Four numbers: x(left), y(bottom), x(right), y(top)
ADPOS	Move the cursor by x,y values.
COLOR	Set color index (ranging from 1 to 16)
GRID	Six number. Draw a grid with x(left), y(bottom), x(right), y(top), gridline distance(x), gridline distance (y)
FONT	Select a font by its index number (from 1 to 6)
XYPOS	Set the cursor to x,y values
LSPAC	Set line spacing in pixels
TSIZE	Set font size in relative value (0.75 is normal)
ROTAT	Set text rotation angles (x, y, z) in degrees (from 0 to 360)
TJUST	Not used. Two values are given. The first number denotes the text justification in x direction, the second number the text justification in y direction
&	The text behind a ampersand is drawn at cursor position (see ADPOS, XYPOS).
;	Comment line

Example

```

;
; DDB logo for Plot programs - file @DDBPTH: DDBLOGO.DxP
;   if file @DDBPRV: DDBLOGO.DxP exist this one is replaced
;
limit 0 300 0 300
adpos 315 30
color 8
line 0,32,32,32,32,26,31,30,33,30,32,26
line 32,26,0,16,32,6,64,16,32,26
line 64,16,68,16,68,31,67,27,69,27,68,31
line 32,6,32,2,0,2,4,3,4,1,0,2
color 3
line 16,14,16,18,18,18,20,17,20,15,18,14,16,14
line 24,14,24,18,26,18,28,17,28,15,26,14,24,14
line 32,14,32,18,35,18,36,17,35,16,32,16,35,16,36,15,35,14,32,14
color 2
line 44,17,43,18,40,18,39,17,40,16,43,16,44,15,43,14,40,14,39,15
line 46,17,46,18,52,18,52,17
line 49,18,49,14
line 48,14,50,14
line 43,5,42,6,40,6,38,5,37,3,38,2,40,2,42,3,42,4,40,4
line 43,2,44,4,44,4,48,4,47,2,48,4,51,4,50,2
line 52,2,54,6,53,4,55,5,57,4,57,3,54,2,53,3
line 58,2,60,6,59,4,64,4,65,6,63,2
;external text file for BIN plot file
limit 0,1000,0,1000
color 1
font 3
    
```

```
tsize .8
tjust 0.1 0.1
lspac 1.3
adpos 0,0
box 0,0,1428,1000
line 900,0,900,1000
line 900,300,1428,300
line 0,850,900,850
adpos 20,930
xypos 0,0
&(1) WATER
&(2) ACETIC ACID
&
adpos 920,930
xypos 0,0
&data set: 13133 VLEDDB
&P = 760.00 [mm Hg]
&
&NRTL
&
&parameters
&A^12~ = 774.4695 [cal/mol]
&A^21~ = 319.5691 [cal/mol]
&a^12~ = 1.4014
&
&Antoine constants [mm Hg, ~o^C]
&
&(1) 8.07126 1730.630 233.426
&(2) 7.55933 1644.050 233.524
adpos 920,320
xypos 0,0
& 3/27/2001
```