Flinders
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Dynamical (e,2e) Studies of Bio-Molecules

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A fact is a simple statement that everyone believes. It is innocent, unless found guilty. A hypothesis is a novel suggestion that no one wants to believe. It is guilty, until found effective.

∼ Edward Teller (1908-2003)

B

Appendix B: GNUPlot Code

B.1 Pyrimidine

B.1.1 Binding Energy Spectrum

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/pybinding.pdf"
unset key

# Labels
set title "Binding Energy Spectrum of Pyrimidine"
set xlabel "Binding Energy (eV)"
set ylabel "Intensity (arb. units)"
set yrange [-0.5:3.5]
set xrange [8:22]

#set label "7b_2"  at first  9.6, first  2.1
set label "11a_1"  at first  10.9, first  2.3
set label "1a_2"  at first  12.4, first  1.2
#set label "10a_1"  at first  13.7, first  3.3
set label "6b_2"  at first  15.0, first  1.9
set label "9a_1"  at first  16.6, first  2
set label "5b_2"  at first  17.5, first  3.0
set label "8a_1"  at first  18.8, first  1.47
#set label "7a_1"  at first  20.6, first  1.2

set label "7b_2 + 2b_1"  at first  9.18, first  2.1
set label "10a_1 + 1b_1"  at first  13.1, first  3.3
set label "7a_1 + 4b_2"  at first  20.23, first  1.2


# Important Details
set label "E_0 = 250 eV"  at first  20, first  3.25
set label "E_{ej} = 20 eV"  at first  20, first  3.10
```

```
30 set label "{/Symbol q}_{sc} = -15^o"  at first  20, first  2.95
31 set label "{/Symbol q}_{ej} = 70^o"  at first  20, first  2.8
32
33
34
35
36 # Styles
37 set style line 1 lt 1 lw 3 linecolor rgb "red"
38 set style line 2 lt 2 lw 1 linecolor rgb "green"
39 set style line 3 lt 1 lw 4 linecolor rgb "blue"
40
41 set style arrow 1 nohead ls 3
42
43
44 # "Arrows"
45 set arrow 1 from 9.83908,1.5 to 9.83908,2 as 1
46 set arrow 2 from 11.1386,1.5 to 11.1386,2.2 as 1
47 set arrow 3 from 12.616,0.6 to 12.616,1.1 as 1
48 set arrow 4 from 13.9379,3.0 to 13.9379,3.2 as 1
49 set arrow 5 from 15.2859,1.2 to 15.2859,1.8 as 1
50 set arrow 6 from 16.8803,1.2 to 16.8803,1.9 as 1
51 set arrow 7 from 17.7305,2.4 to 17.7305,2.9 as 1
52 set arrow 8 from 19.0774,0.87 to 19.0774,1.37 as 1
53 set arrow 9 from 20.896,0.6 to 20.896,1.1 as 1
54
55
56
57
58
59
60
61 # Variables
62 # height = h1,h2,...,h0
63 # centre = c1,c2,...,c0
64 # HWHM = w
65 h1 = 1.2; c1 = 9.8; h2 = 0.3; c2 = 10.5; h3 = 1.0; c3 = 11.3; h4 =
       0.4; c4 = 11.5; h5 = 2.8; c5 = 14.1; h6 = 1.0; c6 = 14.4; h7 =
       0.9; c7 = 15.7; h8 = 2.3; c8 = 17.5; h9 = 0.7; c9 = 17.7; h0 =
       0.4; c0 = 20.6; w = 0.55
66
67 # Math Stuff
68 gauss1(x) = abs ( h1 * exp( -log(2) * ((x - c1) / w) **2) )
69 gauss2(x) = abs ( h2 * exp( -log(2) * ((x - c2) / w) **2) )
70 gauss3(x) = abs ( h3 * exp( -log(2) * ((x - c3) / w) **2) )
71 gauss4(x) = abs ( h4 * exp( -log(2) * ((x - c4) / w) **2) )
72 gauss5(x) = abs ( h5 * exp( -log(2) * ((x - c5) / w) **2) )
73 gauss6(x) = abs ( h6 * exp( -log(2) * ((x - c6) / w) **2) )
74 gauss7(x) = abs ( h7 * exp( -log(2) * ((x - c7) / w) **2) )
75 gauss8(x) = abs ( h8 * exp( -log(2) * ((x - c8) / w) **2) )
76 gauss9(x) = abs ( h9 * exp( -log(2) * ((x - c9) / w) **2) )
```

```
gauss0(x) = abs ( h0 * exp( -log(2) * ((x - c0) / w) **2) )

f(x) = gauss1(x) + gauss2(x) + gauss3(x) + gauss4(x) + gauss5(x) +
    gauss6(x) + gauss7(x) + gauss8(x) + gauss9(x) + gauss0(x)




# Plotting Stuff
fit f(x) 'pybinding' using 1:2:3 via h1, h2, h3, h4, h5, h6, h7, h8
    , h9, h0, c1, c2, c3, c4, c5, c6, c7, c8, c9, c0, w

plot 'pybinding' with errorbars, gauss1(x) with line ls 2, gauss2(x
    ) with line ls 2, gauss3(x) with line ls 2, gauss4(x) with line
     ls 2, gauss5(x) with line ls 2, gauss6(x) with line ls 2,
    gauss7(x) with line ls 2, gauss8(x) with line ls 2, gauss9(x)
    with line ls 2, gauss0(x) with line ls 2, f(x) with line ls 1
```

B.1.2 Triple Differential Cross Sections

Pyrimidine $7b_2$ Orbital

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/py7b2.pdf"
#set output "py7b2.eps"

# Labels
set title "Pyrimidine Triple Differential Cross Section for Orbital
    7b_2"
set xlabel "Ejected Electron Angle (degrees)"
set ylabel "TDCS (10^{-20}m^2eV^{-1}sr^{-1})"
set xrange [0:360]
set yrange [0:0.8]
set encoding iso_8859_1

# Important Details
set label "E_0 = 250 eV"  at first  5, first  0.78
set label "E_{ej} = 20 eV"  at first  5, first  0.75
set label "{/Symbol q}_{sc} = -15^o"  at first  5, first  0.72

# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 head filled ls 3
```

```
set arrow 1 from 68.4,0 to 68.4,0.3 as 1
set arrow 2 from 248.4,0 to 248.4,0.3 as 1
set label "K" at first 65.6, first 0.32 textcolor rgb "blue"
set label "-K" at first 244, first 0.32 textcolor rgb "blue"

plot 'py7b2TDCS' using 1:2:3 with errorbars title "Measured Results
    ", 'py7b2M3DW' using 1:2 with line ls 1 title "7b_2 M3DW"
```

Pyrimidine $10a_1$ Orbital

```
set term postscript eps enhanced size 4in, 8in
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/py10a1.pdf"
#set output "py10a1.eps"

#set size ratio 0.5


# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 2 lt 2 lw 3 linecolor rgb "green"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 head filled ls 3




# Make it a Multi-plot
set multiplot layout 4,1 title "Pyrimidine Triple Differential
    Cross Sections for Orbital 10a_1"
set tmargin 0
set bmargin 0

unset title
unset key

# Labels
set xrange [0:360]
set yrange [0:1.2]


# Important Details
set label "E_0 = 250 eV" at first 300, first 1.1
set label "E_{ej} = 20 eV" at first 300, first 1.03
set label "{/Symbol q}_{sc} = \261 5^o" at first 300, first 0.96




# 5 Degrees
set arrow 1 from 49.9,0 to 49.9,0.5 as 1
```

```
39 set arrow 2 from 229.9,0 to 229.9,0.5 as 1
40 set label "K" at first 47, first 0.55 textcolor rgb "blue"
41 set label "-K" at first 226, first 0.55 textcolor rgb "blue"
42 set format x ""
43 set ylabel " "
44 plot 'py10a1TDCS-5' using 1:2:3 with errorbars title "Measured
       Results", 'py10a1M3DW-5' using 1:2 with line ls 1 title "10a_1
       M3DW"
45
46
47
48 # 10 Degrees
49 unset arrow 1
50 unset arrow 2
51 set arrow 3 from 64,0 to 64,0.5 as 1
52 set arrow 4 from 244,0 to 244,0.5 as 1
53 set ytics 0,0.2,1.0
54 unset label
55 set label "K" at first 61, first 0.55 textcolor rgb "blue"
56 set label "-K" at first 240, first 0.55 textcolor rgb "blue"
57 set label "{/Symbol q}_{sc} = \261 10^o" at first 300, first 1.1
58 set ylabel "TDCS (10^{-20}m^2eV^{-1}sr^{-1})"
59 plot 'py10a1TDCS-10' using 1:2:3 with errorbars title "Measured
       Results", 'py10a1M3DW-10' using 1:2 with line ls 1 title "10a_1
       M3DW"
60
61
62
63 # 15 Degrees
64 unset arrow 3
65 unset arrow 4
66 set arrow 5 from 68.2,0 to 68.2,0.5 as 1
67 set arrow 6 from 248.2,0 to 248.2,0.5 as 1
68 set ytics 0,0.2,1.0
69 unset format
70 unset label
71 set label "K" at first 65, first 0.55 textcolor rgb "blue"
72 set label "-K" at first 244, first 0.55 textcolor rgb "blue"
73 set label "{/Symbol q}_{sc} = \261 15^o" at first 300, first 1.1
74 set xlabel "Ejected Electron Angle (degrees)"
75 set ylabel " "
76 plot 'py10a1TDCS-15' using 1:2:3 with errorbars title "Measured
       Results", 'py10a1M3DW-15' using 1:2 with line ls 1 title "10a_1
       M3DW", 'py10a1M3DW-15_alt' using 1:2 with line ls 2 title "10
       a_1 M3DW"
77
78
79 unset multiplot
```

B.2 α-Tetrahydrofurfuryl Alcohol

B.2.1 Binding Energy Spectrum

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/thfabinding.pdf"
unset key

# Labels
set title "Binding Energy Spectrum of Tetrahydrofurfuryl Alcohol"
set xlabel "Binding Energy (eV)"
set ylabel "Intensity (arb. units)"
set yrange [0:450]
set xrange [8:12]

set label "28a" at first 9.8, first 310
set label "27a" at first 10.80, first 310




# Important Details
set label "E_0 = 250 eV" at first 11.5, first 430
set label "E_{ej} = 20 eV" at first 11.5, first 410
set label "{/Symbol q}_{sc} = -10^o" at first 11.5, first 390
set label "{/Symbol q}_{ej} = 90^o" at first 11.5, first 370




# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 2 lt 2 lw 1 linecolor rgb "green"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 nohead ls 3


# "Arrows"
set arrow 1 from 9.85,100 to 9.85,300 as 1
set arrow 2 from 10.85,200 to 10.85,300 as 1



# Variables
# height = h1,h2,...,h12
# centre = c1,c2,...,c12
# HWHM = w

```

```
46 # PES VALUES
47 h1 = 100; c1 = 9.79; h2 = 150; c2 = 10.93; h3 = 300; c3 = 12.2
48
49
50 # Math Stuff
51 gauss1(x) = abs ( h1 * exp( -log(2) * ((x - c1) / 0.45) **2) )
52 gauss2(x) = abs ( h2 * exp( -log(2) * ((x - c2) / 0.4) **2) )
53 gauss3(x) = abs ( h3 * exp( -log(2) * ((x - c3) / 1.25) **2) )
54
55
56 f(x) = gauss1(x) + gauss2(x) + gauss3(x)
57
58
59 # Plotting Stuff
60 fit f(x) 'thfabinding' using 1:2:3 via h1, h2, c1, c2, c3, h3#, w
61
62 plot 'thfabinding' with errorbars, gauss1(x) with line ls 2, gauss2
       (x) with line ls 2, gauss3(x) with line ls 2, f(x) with line ls
        1
```

B.2.2 Triple Differential Cross Sections

α-Tetrahydrofurfuryl Alcohol 28a Orbital

```
set term postscript eps enhanced size 4in, 8in
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/thfa28a.pdf"
#set output "thfa28a.eps"

#set size ratio 0.5


# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 2 lt 2 lw 3 linecolor rgb "green"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 head filled ls 3




# Make it a Multi-plot
set multiplot layout 4,1 title "Tetrahydrofurfuryl Alcohol Triple
    Differential Cross Sections for Orbital 28a"
set tmargin 0
set bmargin 0

unset title
unset key

# Labels
set xrange [0:360]
set yrange [0:2.2]


# Important Details
set label "E_0 = 250 eV"  at first  300, first  2.05
set label "E_{ej} = 20 eV"  at first  300, first  1.95
set label "{/Symbol q}_{sc} = \261 5^o"  at first  300, first  1.85




# 5 Degrees
set arrow 1 from 49.9,0 to 49.9,0.5 as 1
set arrow 2 from 229.9,0 to 229.9,0.5 as 1
set label "K"  at first  47, first  0.55 textcolor rgb "blue"
set label "-K"  at first  226, first  0.55 textcolor rgb "blue"
set format x ""
set ytics 0,0.2,2.2
set ylabel " "
```

```
45 plot 'thfa28aTDCS' using 1:2:3 with errorbars title "Measured␣
       Results", 'thfa28aM3DW' using 1:2 with line ls 1 title "mee", '
       thfa28aM3DW' using 1:3 with line ls 2 title "nee"
46
47
48
49 # 10 Degrees
50 unset arrow 1
51 unset arrow 2
52 set arrow 3 from 64,0 to 64,0.5 as 1
53 set arrow 4 from 244,0 to 244,0.5 as 1
54 set ytics 0,0.2,2.0
55 unset label
56 set label "K" at first 61, first 0.55 textcolor rgb "blue"
57 set label "-K" at first 240, first 0.55 textcolor rgb "blue"
58 set label "{/Symbol␣q}␣{sc}␣=␣\261␣10^o" at first 300, first
       2.05
59 set ylabel "TDCS␣(10^{-20}m^2eV^{-1}sr^{-1})"
60 plot 'thfa28aTDCS' using 1:4:5 with errorbars title "Measured␣
       Results", 'thfa28aM3DW' using 1:4 with line ls 1 title "mee", '
       thfa28aM3DW' using 1:5 with line ls 2 title "nee"
61
62
63
64 # 15 Degrees
65 unset arrow 3
66 unset arrow 4
67 set arrow 5 from 68.2,0 to 68.2,0.5 as 1
68 set arrow 6 from 248.2,0 to 248.2,0.5 as 1
69 set ytics 0,0.2,2.0
70 unset format
71 unset label
72 set label "K" at first 65, first 0.55 textcolor rgb "blue"
73 set label "-K" at first 244, first 0.55 textcolor rgb "blue"
74 set label "{/Symbol␣q}␣{sc}␣=␣\261␣15^o" at first 300, first
       2.05
75 set xlabel "Ejected␣Electron␣Angle␣(degrees)"
76 set ylabel "␣"
77 plot 'thfa28aTDCS' using 1:6:7 with errorbars title "Measured␣
       Results", 'thfa28aM3DW' using 1:6 with line ls 1 title "mee", '
       thfa28aM3DW' using 1:7 with line ls 2 title "nee"
78
79
80 unset multiplot
```

B.3 Tetrahydrofuran

B.3.1 Binding Energy Spectrum

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/THFbinding.pdf"
unset key

# Labels
set title "Binding Energy Spectrum of Tetrahydrofuran"
set xlabel "Binding Energy (eV)"
set ylabel "Intensity (arb. units)"
set yrange [0:4]
set xrange [7:19]

# Important Details
set label "E_0 = 250 eV" at first 17.5, first 3.9
set label "E_{ej} = 20 eV" at first 17.5, first 3.75
set label "{/Symbol q}_{sc} = -10^o" at first 17.5, first 3.6
set label "{/Symbol q}_{ej} = 75^o" at first 17.5, first 3.45




# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 2 lt 2 lw 1 linecolor rgb "green"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 nohead ls 3


# "Arrows"
set arrow 1 from 9.75,1 to 9.75,1.5 as 1
set arrow 2 from 11.3,1.75 to 11.3,2.25 as 1
set arrow 3 from 12.4,2.7 to 12.4,3.2 as 1
set arrow 4 from 13.9,1.75 to 13.9,2.25 as 1
set arrow 5 from 15.4,2 to 15.4,2.5 as 1
set arrow 6 from 17,2.3 to 17,2.8 as 1
set arrow 7 from 18.8,1.2 to 18.8,1.7 as 1

# Orbital Labels
set label "9b + 12a'" at first 9.3, first 1.6
set label "A" at first 11.2, first 2.35      # Too long - move
    somewhere else
set label "B" at first 12.3, first 3.3       # Too long - move
    somewhere else
set label "C" at first 13.8, first 2.35      # Too long - move
    somewhere else
```

```
43 set label "D" at first 15.3, first 2.6 # Too long - move
       somewhere else
44 set label "5b + 7a'" at first 16.55, first 2.9
45 set label "E" at first 18.7, first 1.8 # Too long - move
       somewhere else
46
47
48 set label "A) 11a + 11a' + 8a''" at first 7.2, first 3.9
49 set label "B) 10a + 10' + 8b + 7a'' + 9a" at first 7.2, first
       3.75
50 set label "C) 6a'' + 7b + 9a' + 6b + 8a" at first 7.2, first 3.6
51 set label "D) 5a'' + 8a'' + 7a" at first 7.2, first 3.45
52 set label "E) 6a + 6a'" at first 7.2, first 3.3
53
54
55 # Variables
56 # height = h1,h2,...,h12
57 # centre = c1,c2,...,c12
58 # HWHM = w
59
60 # (e,2e) VALUES
61 h1 = 1.2; c1 = 9.7; h2 = 0.3; c2 = 11.8; h3 = 1.0; c3 = 12.8; h4 =
       0.4; c4 = 14.3; h6 = 1.0; c6 = 16.6; h7 = 0.9; c7 = 17.7; h8 =
       1; c8 = 19.6; w = 0.55
62
63
64
65
66 # Math Stuff
67 gauss1(x) = abs ( h1 * exp( -log(2) * ((x - c1 + d) / w) **2) )
68 gauss2(x) = abs ( h2 * exp( -log(2) * ((x - c2 + d) / w) **2) )
69 gauss3(x) = abs ( h3 * exp( -log(2) * ((x - c3 + d) / w) **2) )
70 gauss4(x) = abs ( h4 * exp( -log(2) * ((x - c4 + d) / w) **2) )
71 gauss6(x) = abs ( h6 * exp( -log(2) * ((x - c6 + d) / w) **2) )
72 gauss7(x) = abs ( h7 * exp( -log(2) * ((x - c7 + d) / w) **2) )
73 gauss8(x) = abs ( h8 * exp( -log(2) * ((x - c8 + d) / w) **2) )
74
75
76 f(x) = gauss1(x) + gauss2(x) + gauss3(x) + gauss4(x) + gauss6(x) +
       gauss7(x) + gauss8(x)
77
78
79 # Plotting Stuff
80 fit f(x) 'THFbinding' using 4:2:3 via h1, h2, h3, h4, h6, h7, d, w,
        c1, c2, c3, c4, c6, c7, c8#,h8
81
82 plot 'THFbinding' using 4:2:3 with errorbars, gauss1(x) with line
       ls 2, gauss2(x) with line ls 2, gauss3(x) with line ls 2,
       gauss4(x) with line ls 2, gauss6(x) with line ls 2, gauss7(x)
       with line ls 2, gauss8(x) with line ls 2, f(x) with line ls 1
```

B.3.2 Triple Differential Cross Sections

Tetrahydrofuran 9b+12a′ Orbital

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/THFHOMO.pdf"
#set output "THFHOMO.eps"

# Labels
set title "Tetrahydrofuran Triple Differential Cross Section for
    Orbital 9b + 12a'"
set xlabel "Angle (degrees)"
set ylabel "TDCS (10^{-20}m^2eV^{-1}sr^{-1})"
set xrange [0:360]
set yrange [0:3]
set encoding iso_8859_1

# Important Details
set label "E_0 = 250 eV"  at first  5, first  2.9
set label "E_{ej} = 20 eV"  at first  5, first  2.8
set label "{/Symbol q}_{sc} = -5^o"  at first  5, first  2.7

# Styles
set style line 1 lt 2 lw 3 lc 4
set style line 2 lt 3 lw 3 lc 8
set style line 3 lt 1 lw 3 linecolor rgb "red"
set style line 4 lt 2 lw 3 lc 2
set style line 5 lt 3 lw 3 lc 5
set style line 6 lt 1 lw 3 linecolor rgb "blue"


set style line 7 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 head filled ls 7




set arrow 1 from 52.25,0 to 52.25,1.18 as 1
set arrow 2 from 232.94,0 to 232.94,1.18 as 1
set label "K"  at first  50, first  1.23 textcolor rgb "blue"
set label "-K"  at first  228, first  1.23 textcolor rgb "blue"

plot 'THFTDCS' using 1:2:3 with errorbars title "Measured Results",
     'THFM3DW' using 1:3 with line ls 1 title "9b M3DW", 'THFM3DW'
    using 1:2 with line ls 2 title "12a' M3DW", 'THFM3DW' using 1:4
     with line ls 3 title "9b + 12a' M3DW", 'THFDWBA' using 1:3
    with line ls 4 title "9b DWBA", 'THFDWBA' using 1:2 with line
    ls 5 title "12a' DWBA", 'THFDWBA' using 1:4 with line ls 6
    title "9b + 12a' DWBA"
```

B.4 Tetrahydropyran

B.4.1 Binding Energy Spectrum

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/THPbinding.pdf"
unset key

# Labels
set title "Binding Energy Spectrum of Tetrahydropyran"
set xlabel "Binding Energy (eV)"
set ylabel "Intensity (arb. units)"
set yrange [0:300]
set xrange [7:18]


# Important Details
set label "E_0 = 250 eV" at first 16.6, first 290
set label "E_{ej} = 20 eV" at first 16.6, first 280
set label "{/Symbol q}_{sc} = -10^o" at first 16.6, first 270
set label "{/Symbol q}_{ej} = 75^o" at first 16.6, first 260


# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 2 lt 2 lw 1 linecolor rgb "green"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 nohead ls 3


# "Arrows"
set arrow 1 from 9.3,60 to 9.3,110 as 1
set arrow 2 from 11.3,160 to 11.3,220 as 1
set arrow 3 from 12.6,180 to 12.6,260 as 1
set arrow 4 from 13.65,220 to 13.65,275 as 1
set arrow 5 from 15.3,235 to 15.3,275 as 1
set arrow 6 from 16.7,160 to 16.7,220 as 1

# Orbital Labels
set label "15a'" at first 9.1, first 115
set label "14a' + 9a'" at first 10.7, first 225
set label "13a' + 8a''" at first 12, first 265
set label "A" at first 13.57, first 280      # Too Long!
set label "B" at first 15.20, first 280      #Too Long!
set label "9a'" at first 16.55, first 225


set label "A) 12a' + 7a'' + 6a''" at first 7.2, first 290
```

```
46 set label "B) 11a' + 10a' + 5a''"  at first  7.2, first  280
47
48
49
50 # Variables
51 # height = h1,h2,...,h6
52 # centre = c1,c2,...,c6
53 # HWHM = w
54
55 # (e,2e) VALUES
56 h1 = 50; c1 = 9.46; h2 = 130; c2 = 11.3; h3 = 130; c3 = 12.3; h4 =
       160; c4 = 13.6; h5 = 200; c5 = 15.5; h6 = 130; c6 = 16.6; w =
       0.55
57
58
59
60
61 # Math Stuff
62 gauss1(x) = abs ( h1 * exp( -log(2) * ((x - c1) / w + d) **2) )
63 gauss2(x) = abs ( h2 * exp( -log(2) * ((x - c2) / w + d) **2) )
64 gauss3(x) = abs ( h3 * exp( -log(2) * ((x - c3) / w + d) **2) )
65 gauss4(x) = abs ( h4 * exp( -log(2) * ((x - c4) / w + d) **2) )
66 gauss5(x) = abs ( h5 * exp( -log(2) * ((x - c5) / w + d) **2) )
67 gauss6(x) = abs ( h6 * exp( -log(2) * ((x - c6) / w + d) **2) )
68
69
70 f(x) = gauss1(x) + gauss2(x) + gauss3(x) + gauss4(x) + gauss5(x) +
       gauss6(x)
71
72
73 # Plotting Stuff
74 fit f(x) 'THPbinding' using 4:2:3 via h1, h2, h3, h4, h5, h6, c1,
       c2, c3, c4, c5, c6, d#, w
75
76 plot 'THPbinding' using 4:2:3 with errorbars, gauss1(x) with line
       ls 2, gauss2(x) with line ls 2, gauss3(x) with line ls 2,
       gauss4(x) with line ls 2, gauss5(x) with line ls 2, gauss6(x)
       with line ls 2, f(x) with line ls 1
```

B.4.2 Triple Differential Cross Sections

Tetrahydropyran 15a′ Orbital

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - - ../Thesis/Plots/THP15a.pdf"
#set output "THP15a.eps"

# Labels
set title "Tetrahydropyran Triple Differential Cross Section for
    Orbital 15a'"
set xlabel "Angle (degrees)"
set ylabel "TDCS (10^{-20}m^2eV^{-1}sr^{-1})"
set xrange [0:360]
set yrange [0:1.6]
set encoding iso_8859_1

# Important Details
set label "E_0 = 250 eV" at first 5, first 1.55
set label "E_{ej} = 20 eV" at first 5, first 1.5
set label "{/Symbol q}_{sc} = 5^o" at first 5, first 1.45

# Styles
set style line 1 lt 2 lw 3 lc 4
set style line 2 lt 3 lw 3 lc 8
set style line 3 lt 1 lw 3 linecolor rgb "red"
set style line 4 lt 2 lw 3 lc 2
set style line 5 lt 3 lw 3 lc 5
set style line 6 lt 1 lw 3 linecolor rgb "blue"


set style line 7 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 head filled ls 7







set arrow 1 from 52.25,0 to 52.25,0.4 as 1
set arrow 2 from 232.94,0 to 232.94,0.4 as 1
set label "K" at first 50, first 0.5 textcolor rgb "blue"
set label "-K" at first 228, first 0.5 textcolor rgb "blue"

plot 'THP15a' using 1:2:3 with errorbars title "Measured Results",
    'THPM3DW' using 1:2 with line ls 3 title "15a' M3DW"
```

B.5 1,4 - Dioxane

B.5.1 Binding Energy Spectrum

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - ../Thesis/Plots/dioxbinding.pdf"
unset key

# Labels
set title "Binding Energy Spectrum of 1,4-Dioxane"
set xlabel "Binding Energy (eV)"
set ylabel "Intensity (arb. units)"
set yrange [0:2.5]
set xrange [6:20]

set label "8a_g" at first 9.12, first 1.0
set label "7a_g" at first 10.42, first 1.5
set label "7b_u" at first 10.95, first 1.7
set label "5a_u" at first 12.32, first 2.0
set label "4b_g + 6b_u" at first 12.68, first 2.2
set label "4a_u" at first 13.85, first 2.0
set label "6a_g" at first 15.12, first 1.7
set label "3a_u + 3b_g" at first 15.44, first 2.3
#set label "5b_u" at first 16.37, first 2.1
set label "5b_u + 5a_g" at first 16.34, first 1.9


# Important Details
set label "E_0 = 250 eV" at first 18, first 2.4
set label "E_{ej} = 20 eV" at first 18, first 2.3
set label "{/Symbol q}_{sc} = -10^o" at first 18, first 2.2
set label "{/Symbol q}_{ej} = 75^o" at first 18, first 2.1




# Styles
set style line 1 lt 1 lw 3 linecolor rgb "red"
set style line 2 lt 2 lw 1 linecolor rgb "green"
set style line 3 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 nohead ls 3


# "Arrows"
#set arrow 1 from 9.37,0.42 to 9.37,0.95 as 1
#set arrow 2 from 10.67,0.76 to 10.67,1.45 as 1
#set arrow 3 from 11.22,0.63 to 11.22,1.65 as 1
#set arrow 4 from 12.57,0.92 to 12.57,1.95 as 1
```

```
46 #set arrow 5 from 13.34,0.96 to 13.34,2.15 as 1
47 #set arrow 6 from 14.05,1.02 to 14.05,1.95 as 1
48 #set arrow 7 from 15.37,0.85 to 15.37,1.65 as 1
49 #set arrow 8 from 16.1,0.64 to 16.1,2.25 as 1
50 #set arrow 10 from 17,1.2 to 17,1.85 as 1
51
52
53 set arrow 1 from 9.37,0.75 to 9.37,0.95 as 1
54 set arrow 2 from 10.67,1.25 to 10.67,1.45 as 1
55 set arrow 3 from 11.22,1.45 to 11.22,1.65 as 1
56 set arrow 4 from 12.57,1.75 to 12.57,1.95 as 1
57 set arrow 5 from 13.34,1.95 to 13.34,2.15 as 1
58 set arrow 6 from 14.05,1.75 to 14.05,1.95 as 1
59 set arrow 7 from 15.37,1.45 to 15.37,1.65 as 1
60 set arrow 8 from 16.1,2.05 to 16.1,2.25 as 1
61 set arrow 10 from 17,1.65 to 17,1.85 as 1
62
63
64
65
66
67 # Variables
68 # height = h1,h2,...,h12
69 # centre = c1,c2,...,c12
70 # HWHM = w
71
72 # THEORETICAL VALUES
73 #h1 = 1.2; c1 = 10.56; h2 = 0.3; c2 = 12.08; h3 = 1.0; c3 = 12.36;
       h4 = 0.4; c4 = 14.03; h5 = 2.8; c5 = 14.06; h6 = 1.0; c6 =
       14.64; h7 = 0.9; c7 = 15.21; h8 = 2.3; c8 = 17.28; h9 = 0.7; c9
        = 17.35; h10 = 0.4; c10 = 17.73; h11 = 0.4; c11 = 17.8; h12 =
       0.4; c12 = 18.96; w = 0.55
74
75 # PES VALUES
76 h1 = 1.2; c1 = 9.37; h2 = 0.3; c2 = 10.67; h3 = 1.0; c3 = 11.2; h4
       = 0.4; c4 = 12.57; h6 = 1.0; c6 = 13.34; h7 = 0.9; c7 = 14.05;
       h8 = 2.3; c8 = 15.37; h9 = 0.7; c9 = 16.1; h12 = 0.4; c12 = 17;
        w = 0.55
77
78
79
80
81 # Math Stuff
82 gauss1(x) = abs ( h1 * exp( -log(2) * ((x - c1 + d) / w) **2) )
83 gauss2(x) = abs ( h2 * exp( -log(2) * ((x - c2 + d) / w) **2) )
84 gauss3(x) = abs ( h3 * exp( -log(2) * ((x - c3 + d) / w) **2) )
85 gauss4(x) = abs ( h4 * exp( -log(2) * ((x - c4 + d) / w) **2) )
86 gauss6(x) = abs ( h6 * exp( -log(2) * ((x - c6 + d) / w) **2) )
87 gauss7(x) = abs ( h7 * exp( -log(2) * ((x - c7 + d) / w) **2) )
88 gauss8(x) = abs ( h8 * exp( -log(2) * ((x - c8 + d) / w) **2) )
```

```
89 gauss9(x) = abs ( h9 * exp( -log(2) * ((x - c9 + d) / w) **2) )
90 gauss12(x) = abs ( h12 * exp( -log(2) * ((x - c12 + d) / w) **2) )
91
92 f(x) = gauss1(x) + gauss2(x) + gauss3(x) + gauss4(x) + gauss6(x) +
       gauss7(x) + gauss8(x) + gauss9(x) +  gauss12(x)
93
94
95
96
97 # Plotting Stuff
98 fit f(x) 'dioxbinding' using 1:2:3 via h1, h2, h3, h4, h6, h7, h8,
       h9, h12, d#, c1, c2, c3, c4, c6, c7, c8, c9, c12#, w
99
100 plot 'dioxbinding' with errorbars, gauss1(x) with line ls 2, gauss2
       (x) with line ls 2, gauss3(x) with line ls 2, gauss4(x) with
       line ls 2, gauss6(x) with line ls 2, gauss7(x) with line ls 2,
       gauss8(x) with line ls 2, gauss9(x) with line ls 2, gauss12(x)
       with line ls 2, f(x) with line ls 1
```

B.5.2 Triple Differential Cross Sections

1,4-Dioxane $8a_g$ Orbital

```
set term postscript eps enhanced
set output "| ps2pdf -dEPSCrop - - ../Thesis/Plots/diox8ag.pdf"
#set output "diox8ag.eps"

# Labels
set title "1,4-Dioxane Triple Differential Cross Section for
    Orbital 8a_g"
set xlabel "Angle (degrees)"
set ylabel "TDCS (10^{-20}m^2eV^{-1}sr^{-1})"
set xrange [0:360]
set yrange [0:1]
set encoding iso_8859_1

# Important Details
set label "E_0 = 250 eV"  at first  5, first  .95
set label "E_{ej} = 20 eV"  at first  5, first  .92
set label "{/Symbol q}_{sc} = 5^o"  at first  5, first  .89

# Styles
set style line 1 lt 2 lw 3 lc 4
set style line 2 lt 3 lw 3 lc 8
set style line 3 lt 1 lw 3 linecolor rgb "red"
set style line 4 lt 2 lw 3 lc 2
set style line 5 lt 3 lw 3 lc 5
set style line 6 lt 1 lw 3 linecolor rgb "blue"


set style line 7 lt 1 lw 4 linecolor rgb "blue"

set style arrow 1 head filled ls 7




set arrow 1 from 50.91,0 to 50.91,0.18 as 1
set arrow 2 from 230.91,0 to 230.91,0.18 as 1
set label "K"  at first  50, first  0.20 textcolor rgb "blue"
set label "-K"  at first  226, first  0.20 textcolor rgb "blue"

plot 'diox8ag' using 1:2:3 with errorbars title "Measured Results",
     'diox8agM3DW' using 1:2 with line ls 3 title "8a_g M3DW"
```