> #Diffusion in Li3N;

```
restart;
with(Optimization);
 with(Statistics);
 with(Plot);
 with(plots);
```

[*ImportMPS*, *Interactive*, *LPSolve*, *LSSolve*, *Maximize*, *Minimize*, *NLPSolve*, *QPSolve*]

[*AbsoluteDeviation*, *AgglomeratedPlot*, *AreaChart*, *AutoCorrelation*, *BarChart*, *Bootstrap*, *BoxPlot*, *BubblePlot*, *CDF*, *CGF*, *CentralMoment*, *CharacteristicFunction*, *ChiSquareGoodnessOfFitTest*, *ChiSquareIndependenceTest*, *ChiSquareSuitableModelTest*, *ColumnGraph*, *Correlation*, *CorrelationMatrix*, *Count*, *CountMissing*, *Covariance*, *CovarianceMatrix*, *CrossCorrelation*, *Cumulant*, *CumulantGeneratingFunction*, *CumulativeDistributionFunction*, *CumulativeProduct*, *CumulativeSum*, *CumulativeSumChart*, *DataSummary*, *Decile*, *DensityPlot*, *DiscreteValueMap*, *Discretize*, *Distribution*, *ErrorPlot*, *EvaluateToFloat*, *Excise*, *ExpectedValue*, *ExponentialFit*, *ExponentialSmoothing*, *FailureRate*, *FisherInformation*, *Fit*, *FivePointSummary*, *FrequencyPlot*, *FrequencyTable*, *GeometricMean*, *HarmonicMean*, *HazardRate*, *Histogram*, *Information*, *InteractiveDataAnalysis*, *InterquartileRange*, *InverseSurvivalFunction*, *Join*, *KernelDensity*, *KernelDensityPlot*, *KernelDensitySample*, *Kurtosis*, *Likelihood*, *LikelihoodRatioStatistic*, *LineChart*, *LinearFilter*, *LinearFit*, *LogLikelihood*, *LogarithmicFit*, *MGF*, *MLE*, *MakeProcedure*, *MaximumLikelihoodEstimate*, *Mean*, *MeanDeviation*, *Median*, *MedianDeviation*, *MillsRatio*, *Mode*, *Moment*, *MomentGeneratingFunction*, *MovingAverage*, *MovingMedian*, *MovingStatistic*, *NonlinearFit*, *NormalPlot*, *OneSampleChiSquareTest*, *OneSampleTTest*, *OneSampleZTest*, *OneWayANOVA*, *OrderByRank*, *OrderStatistic*, *PDF*, *Percentile*, *PieChart*, *PointPlot*, *PolynomialFit*, *PowerFit*, *Probability*, *ProbabilityDensityFunction*, *ProbabilityFunction*, *ProbabilityPlot*, *ProfileLikelihood*, *ProfileLogLikelihood*, *QuadraticMean*, *Quantile*, *QuantilePlot*, *Quartile*, *RandomVariable*, *Range*, *Rank*, *Remove*, *RemoveInRange*, *RemoveNonNumeric*, *Sample*, *ScatterPlot*, *ScatterPlot3D*, *Score*, *Select*, *SelectInRange*, *SelectNonNumeric*, *ShapiroWilkWTest*, *Shuffle*, *Skewness*, *Sort*, *SplitByColumn*, *StandardDeviation*, *StandardError*, *StandardizedMoment*, *SunflowerPlot*, *Support*, *SurfacePlot*, *SurvivalFunction*, *SymmetryPlot*, *Tally*, *TallyInto*, *Trim*, *TrimmedMean*, *TwoSampleFTest*, *TwoSamplePairedTTest*, *TwoSampleTTest*, *TwoSampleZTest*, *Variance*, *Variation*, *WeightedMovingAverage*, *Winsorize*, *WinsorizedMean*]

[*ColorRange*, *DualAxisPlot*, *FormatText*, *GetAdaptiveOptions*, *IsCoordinateSystem*, *IsOption*, *LogPlot2D*, *MergeAXIS*, *ModuleApply*, *Plot2D*, *Plot3D*, *PlotArray*, *PointPlot*, *PolarPlot*, *PolygonPlot*, *Preprocess*, *ProcessUnits*, *SetColors*, *SetColours*, *Structure*, *TextPlot*,

TranslateOptions, *Utilities*, *VerifyAdaptiveOptions*]

[*animate*, *animate3d*, *animatecurve*, *arrow*, *changecoords*, *complexplot*, *complexplot3d*, *conformal*, *conformal3d*, *contourplot*, *contourplot3d*, *coordplot*, *coordplot3d*, *densityplot*, *display*, *dualaxisplot*, *fieldplot*, *fieldplot3d*, *gradplot*, *gradplot3d*, *implicitplot*, *implicitplot3d*, *inequal*, *interactive*, *interactiveparams*, *intersectplot*, *listcontplot*, *listcontplot3d*, *listdensityplot*, *listplot*, *listplot3d*, *loglogplot*, *logplot*, *matrixplot*, *multiple*, *odeplot*, *pareto*, *plotcompare*, *pointplot*, *pointplot3d*, *polarplot*, *polygonplot*, *polygonplot3d*, *polyhedra_supported*, *polyhedraplot*, *rootlocus*, *semilogplot*, *setcolors*, *setoptions*, *setoptions3d*, *spacecurve*, *sparsematrixplot*, *surfdata*, *textplot*, *textplot3d*, *tubeplot*] **(1)**

```
g := 1655;
T := 1.0267e-2;
d := 1.2e-3;
t := 4.2e-4;
Gi := Vector([50, 120, 190, 261, 331, 401, 471, 541, 611, 681, 751, 822, 892, 962, 1030, 1100], datatype = float);
Ai := Vector([1.0, 0.983, 0.892, 0.824, 0.735, 0.619, 0.548, 0.488, 0.4, 0.366, 0.311, 0.293, 0.267, 0.242, 0.195, 0.184], datatype = float);
Plot2D(Gi, Ai, style = point, view = 0..1.05);
```

1655

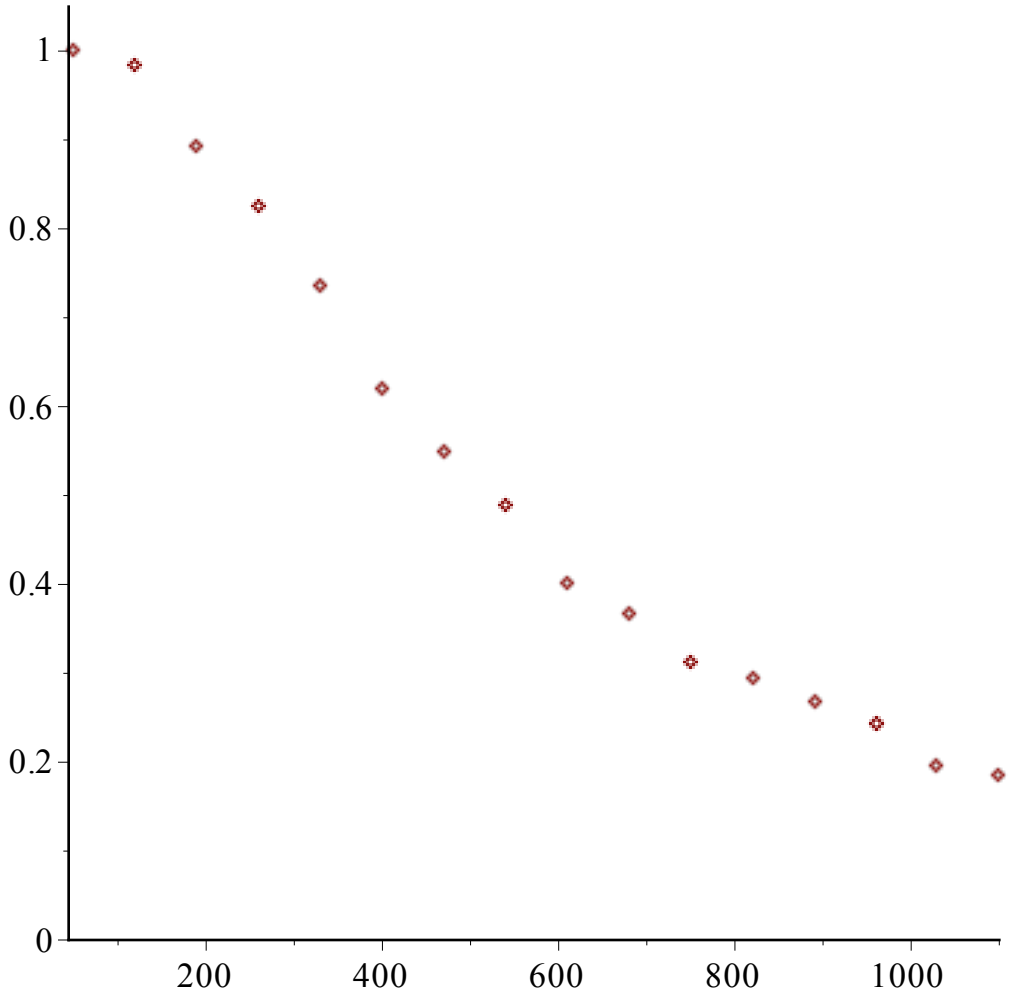
0.010267

0.0012

0.00042

$$\begin{bmatrix} 1 .. 16\ Vector_{column} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$

$$\begin{bmatrix} 1 .. 16\ Vector_{column} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$



$$A := (\mathrm{D}, G, I0, I1) \rightarrow I0 \cdot \exp\left(-\mathrm{D} \cdot (2 \cdot \mathrm{Pi} \cdot g \cdot G \cdot d)^2 \cdot \left(\mathrm{T} + \frac{2 \cdot \mathrm{d}}{3} + \frac{3 \cdot t}{4} \right) \cdot 10^{-5} \right) + I1;$$

$$ChiSquare := (\mathrm{D}, I0, I1) \rightarrow add\left((A(\mathrm{D}, Gi[i], I0, I1) - Ai[i])^2, i = 1..16 \right);$$

$$Ab := (DZ, DXY, G, I0, I1) \rightarrow evalf\left(I0 \cdot Int\left(\exp\left(-\left(DZ \cdot (\cos(x))^2 + DXY \cdot (\sin(x))^2 \right) \cdot (2 \cdot \mathrm{Pi} \cdot g \cdot G \cdot d)^2 \cdot \left(\mathrm{T} + \frac{2 \cdot \mathrm{d}}{3} + \frac{3 \cdot t}{4} \right) \cdot 10^{-5} \right) \cdot \sin(x), x = 0..1.570796327 \right) + I1 \right);$$

$$ChiSquareb := (DZ, DXY, I0, I1) \rightarrow add\left((Ab(DZ, DXY, Gi[i], I0, I1) - Ai[i])^2, i = 1..16 \right);$$

$$(\mathrm{D}, G, I0, I1) \rightarrow I0 \, \mathrm{e}^{-\frac{1}{25000} \mathrm{D} \pi^2 g^2 G^2 d^2 \left(T + \frac{2}{3} d + \frac{3}{4} t \right)} + I1$$

$$(\mathrm{D}, I0, I1) \rightarrow add\left(\left(A\left(\mathrm{D}, Gi_i, I0, I1 \right) - Ai_i \right)^2, i = 1..16 \right)$$

$$(DZ, DXY, G, I0, I1) \rightarrow evalf\left(I0 \left(\right. \right.$$

$$\int_0^{1.570796327} e^{-\frac{1}{25000}\left(DZ\cos(x)^2 + DXY\sin(x)^2\right)\pi^2 g^2 G^2 d^2\left(T+\frac{2}{3}d+\frac{3}{4}t\right)\sin(x)}\,dx\Bigg) + I1\Bigg)$$

$$(DZ, DXY, I0, I1) \rightarrow add\left(\left(Ab\left(DZ, DXY, Gi_i, I0, I1\right) - Ai_i\right)^2, i = 1..16\right) \quad \textbf{(2)}$$

$Solution := Minimize(ChiSquare(\mathrm{D}, I0, I1), \mathrm{D} = 0..1.0, I0 = 0.5..1.5, I1 = 0..0.2, initialpoint = \{\mathrm{D} = 0.07, I0 = 1.0, I1 = 0\}, variables = [\mathrm{D}, I0, I1]);$

$[0.00448576048347442986, [\mathrm{D} = 0.206562419061777, I0 = 0.799188244023435, I1 = 0.203219188200893]]$ **(3)**

$rhs\left(\left(Solution_2\right)_1\right);$

$$0.206562419061777 \quad \textbf{(4)}$$

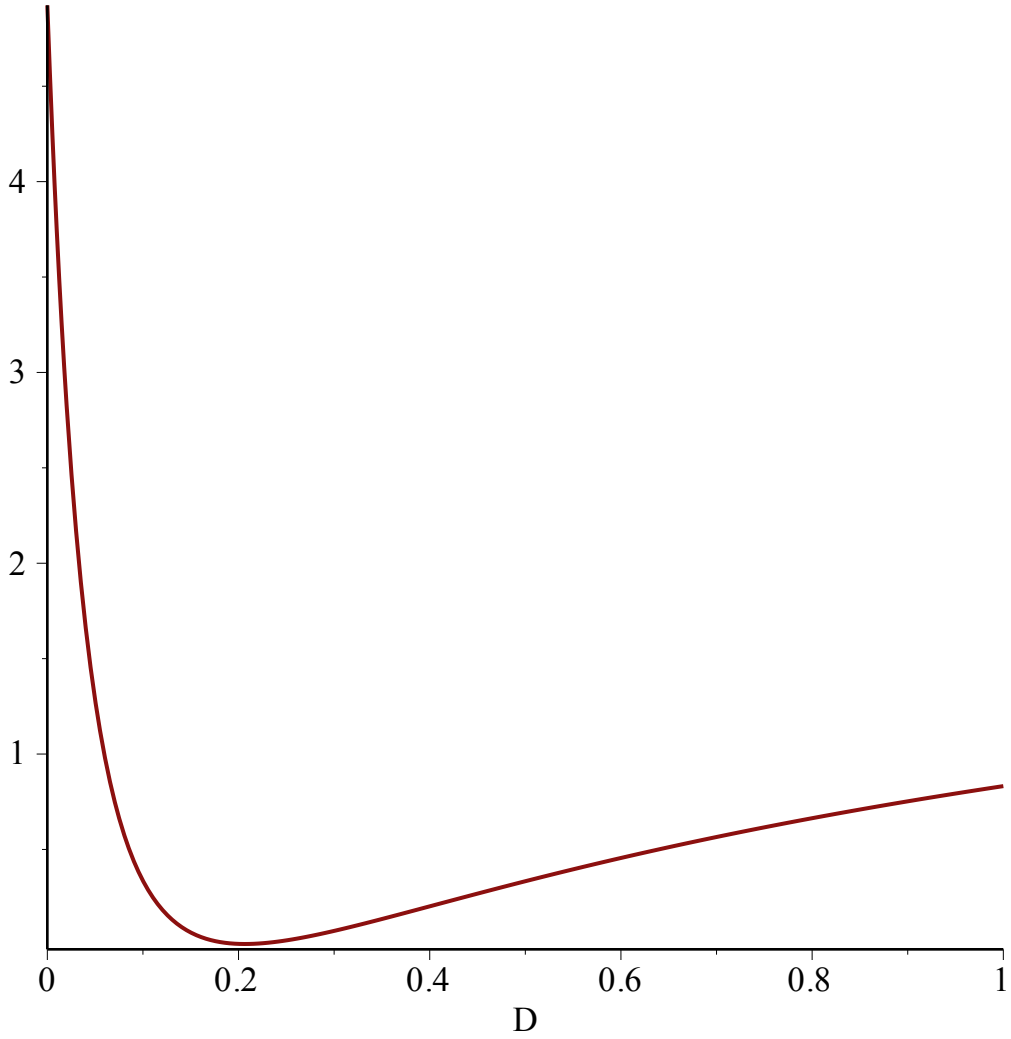
$Plot2D\left(ChiSquare\left(\mathrm{D}, rhs\left(\left(Solution_2\right)_2\right), rhs\left(\left(Solution_2\right)_3\right)\right), \mathrm{D} = 0..1\right);$

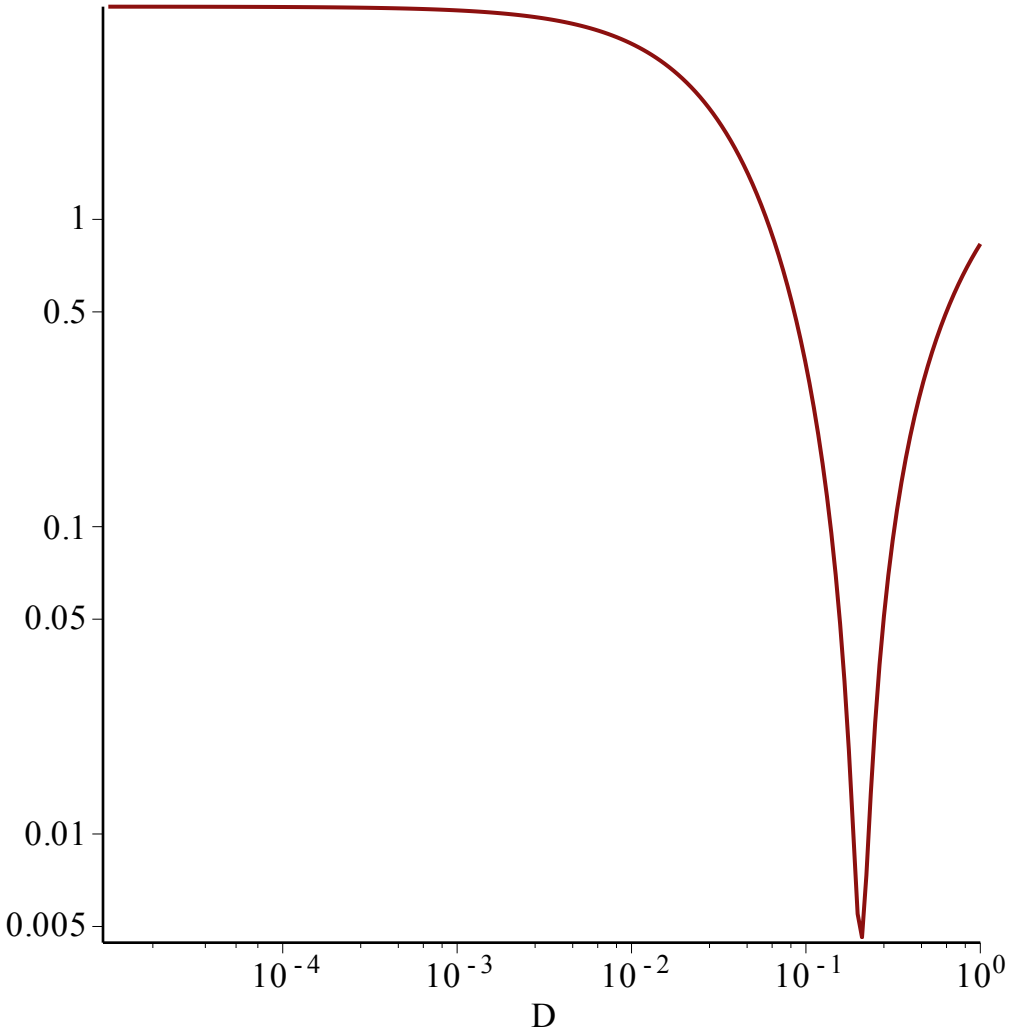
$\mathrm{loglogplot}\left(ChiSquare\left(\mathrm{D}, rhs\left(\left(Solution_2\right)_2\right), rhs\left(\left(Solution_2\right)_3\right)\right), \mathrm{D} = 1e-5..1\right);$

$a := Plot2D\left(A\left(rhs\left(\left(Solution_2\right)_1\right), G, rhs\left(\left(Solution_2\right)_2\right), rhs\left(\left(Solution_2\right)_3\right)\right), G = 0..1200, color = blue\right);$

$b := Plot2D(Gi, Ai, style = point, view = 0..1.05);$

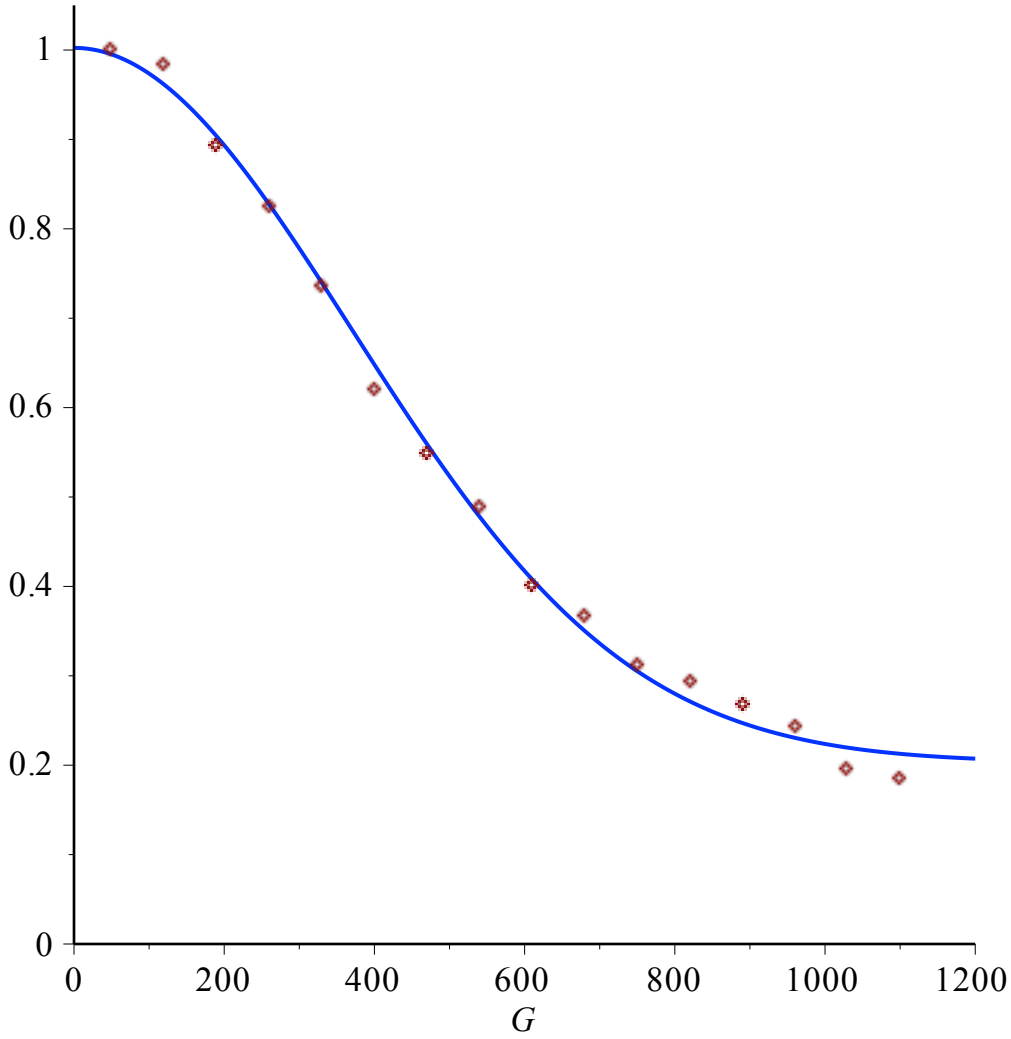
$display(\{a, b\});$





PLOT(...)

PLOT(...)

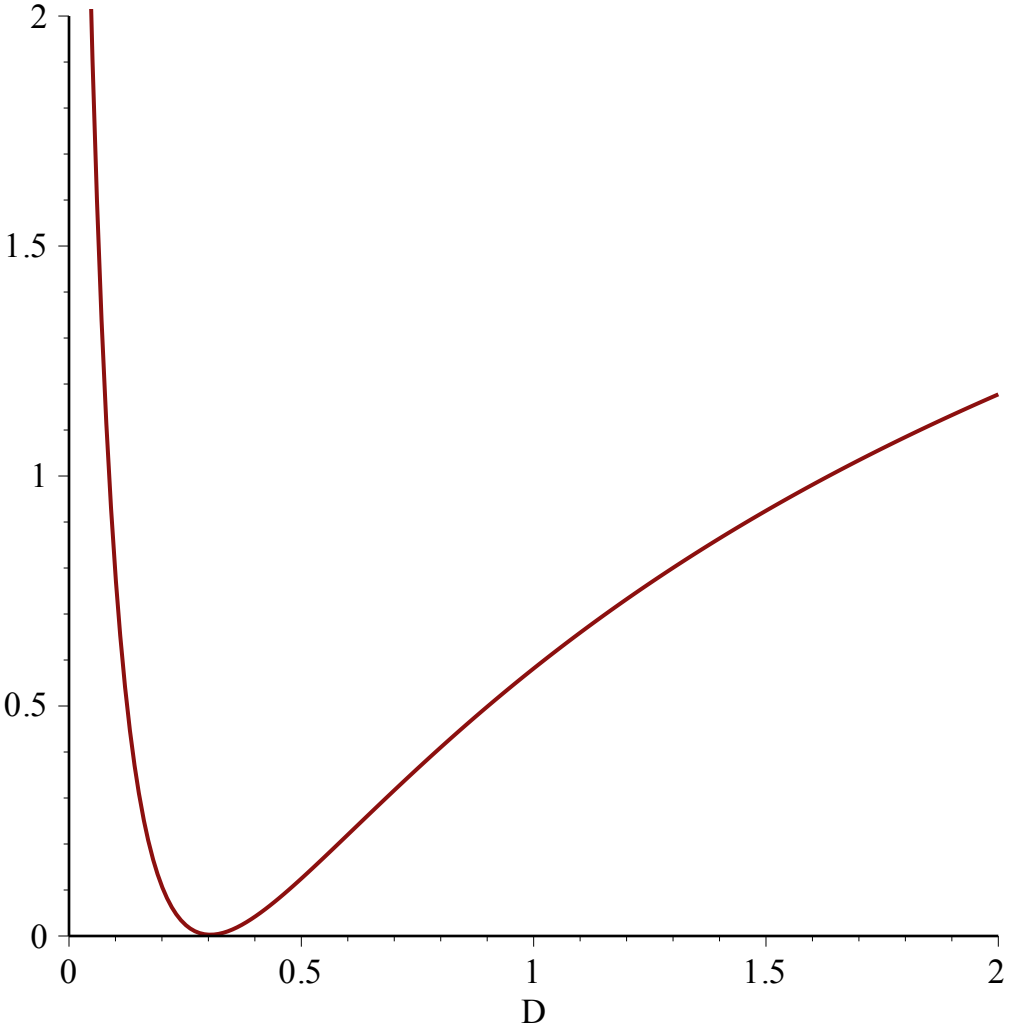


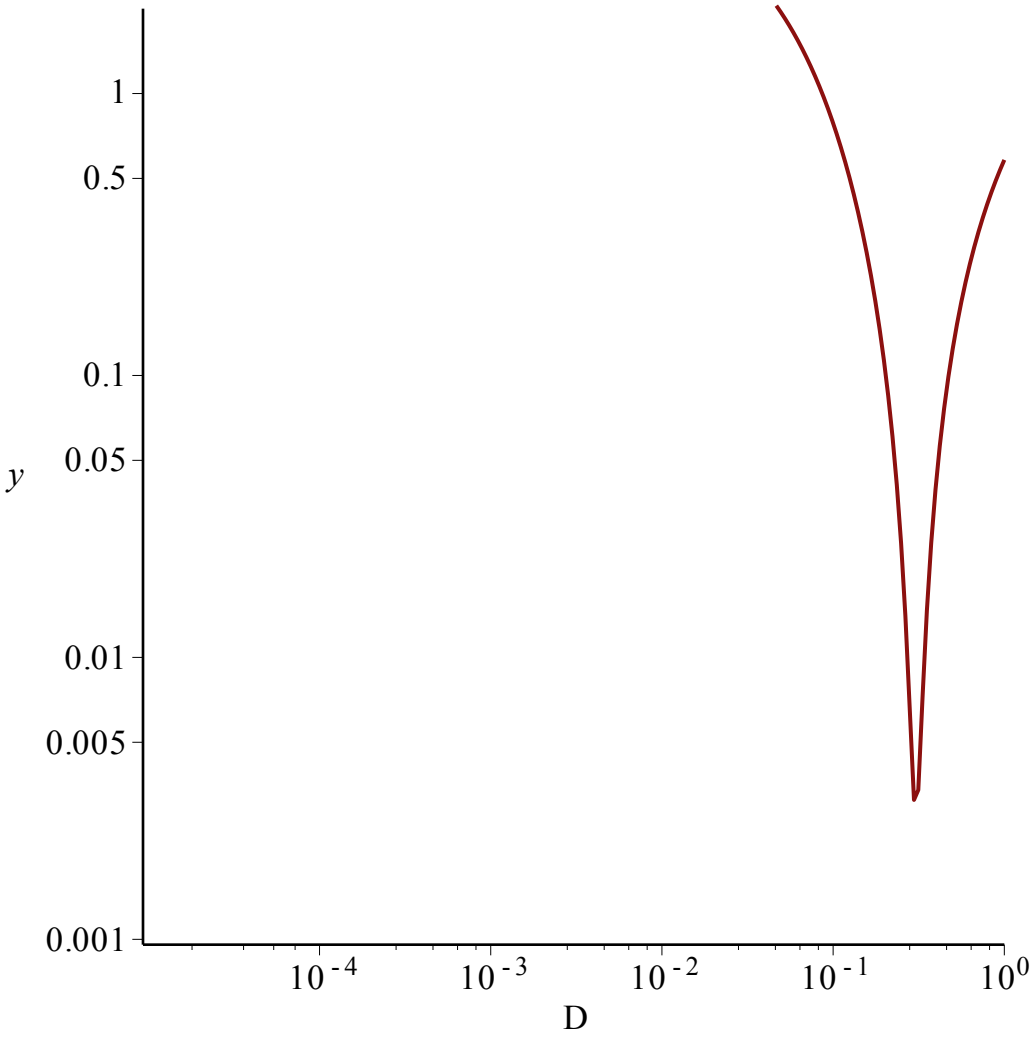
Solutionb := *Minimize*(*ChiSquareb*(0.0, D, *I0*, *I1*), D = 0 ..1.0, *I0* = 0.5 ..1.5, *I1* = 0 ..1, *initialpoint* = {D = 0.07, *I0* = 1.0, *I1* = 0}, *variables* = [D, *I0*, *I1*]);

Plot2D(*ChiSquareb*(0, D, *rhs*((*Solutionb*$_2$)$_2$), *rhs*((*Solutionb*$_2$)$_3$)), D = 0 ..2);

loglogplot(*ChiSquareb*(0, D, *rhs*((*Solutionb*$_2$)$_2$), *rhs*((*Solutionb*$_2$)$_3$)), D = 1e-5 ..1, *y* = 1e-3 ..2);

[0.00278248156854856528, [D = 0.304151766207583, *I0* = 0.881112571033841, *I1* = 0.128545786444715]]





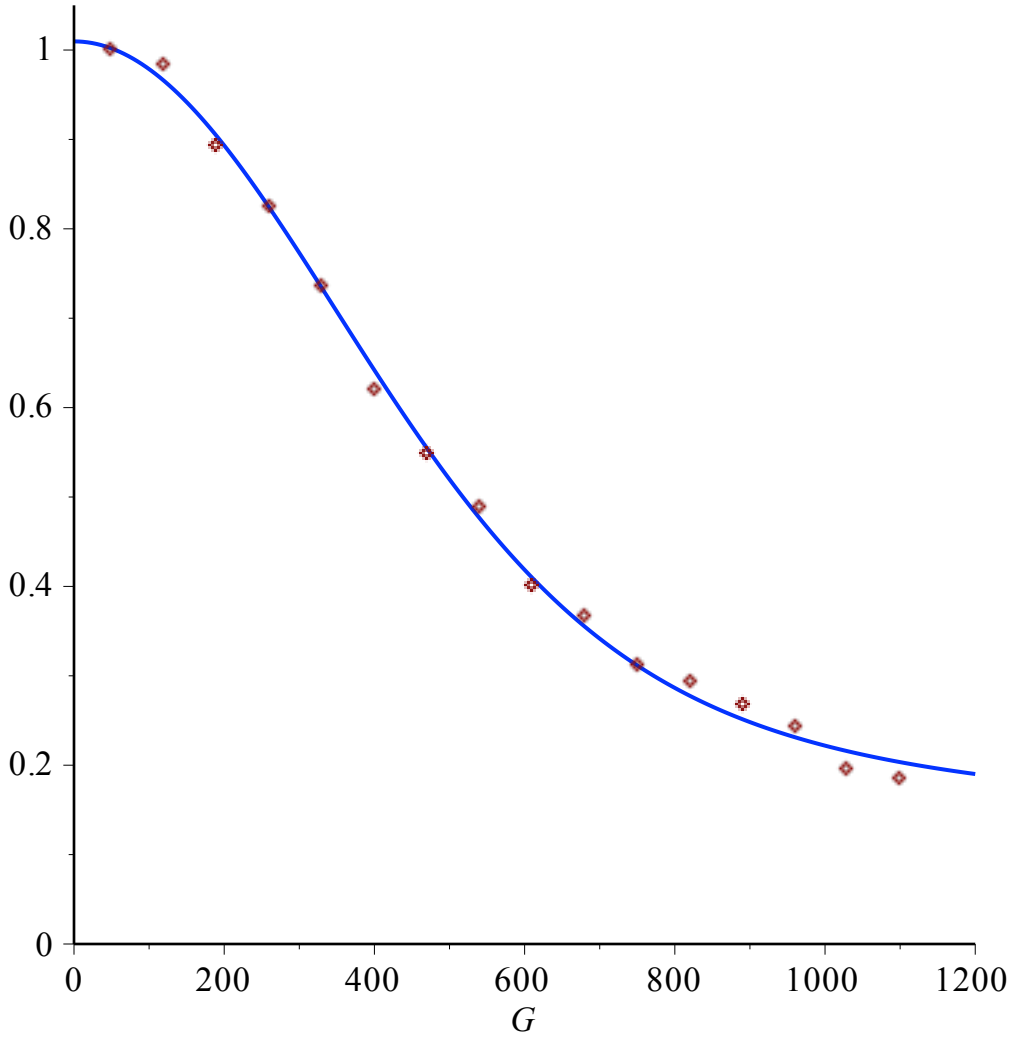
$a := Plot2D\left(Ab\left(0.0, rhs\left(\left(Solutionb_2\right)_1\right), G, rhs\left(\left(Solutionb_2\right)_2\right), rhs\left(\left(Solutionb_2\right)_3\right)\right), G = 0..1200, color = blue\right);$

$b := Plot2D(Gi, Ai, style = point, view = 0..1.05);$

$display(\{a, b\});$

$PLOT(...)$

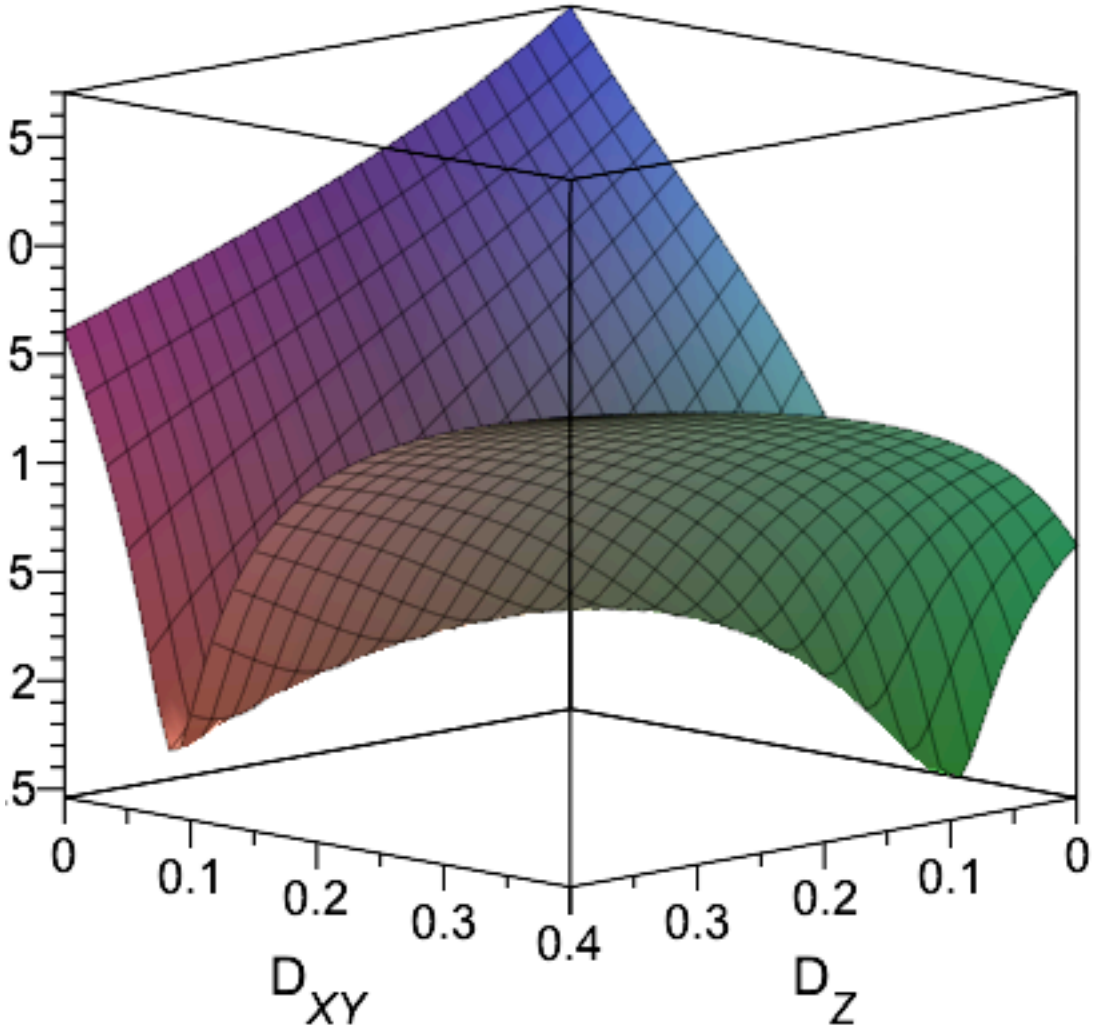
$PLOT(...)$



$Solutionc := Minimize(ChiSquareb(Dpar, Dort, I0, I1), Dpar = 0..1.0, Dort = 0..1.0, I0 = 0.5..1.5, I1 = 0..1, initialpoint = \{Dpar = 0.01, Dort = 0.11, I0 = 1.0, I1 = 0\}, variables = [Dpar, Dort, I0, I1]);$

$$[0.00278248156849532358, [Dpar = 8.04779426142891\ 10^{-8}, Dort = 0.304151627344438, I0 = 0.881112501699741, I1 = 0.128545762295655]] \quad \textbf{(5)}$$

try
$plotsetup(default);$
$print(plot3d(\log10(ChiSquareb(D_Z, D_{XY}, rhs((Solutionc_2)_3), rhs((Solutionc_2)_4))), D_Z = 0..0.4, D_{XY} = 0..0.4, axes = boxed, orientation = [45, 80, 0], font = [Arial, default, 14], labelfont = [Arial, default, 16]));$
finally
$plotsetup(default);$
end try;



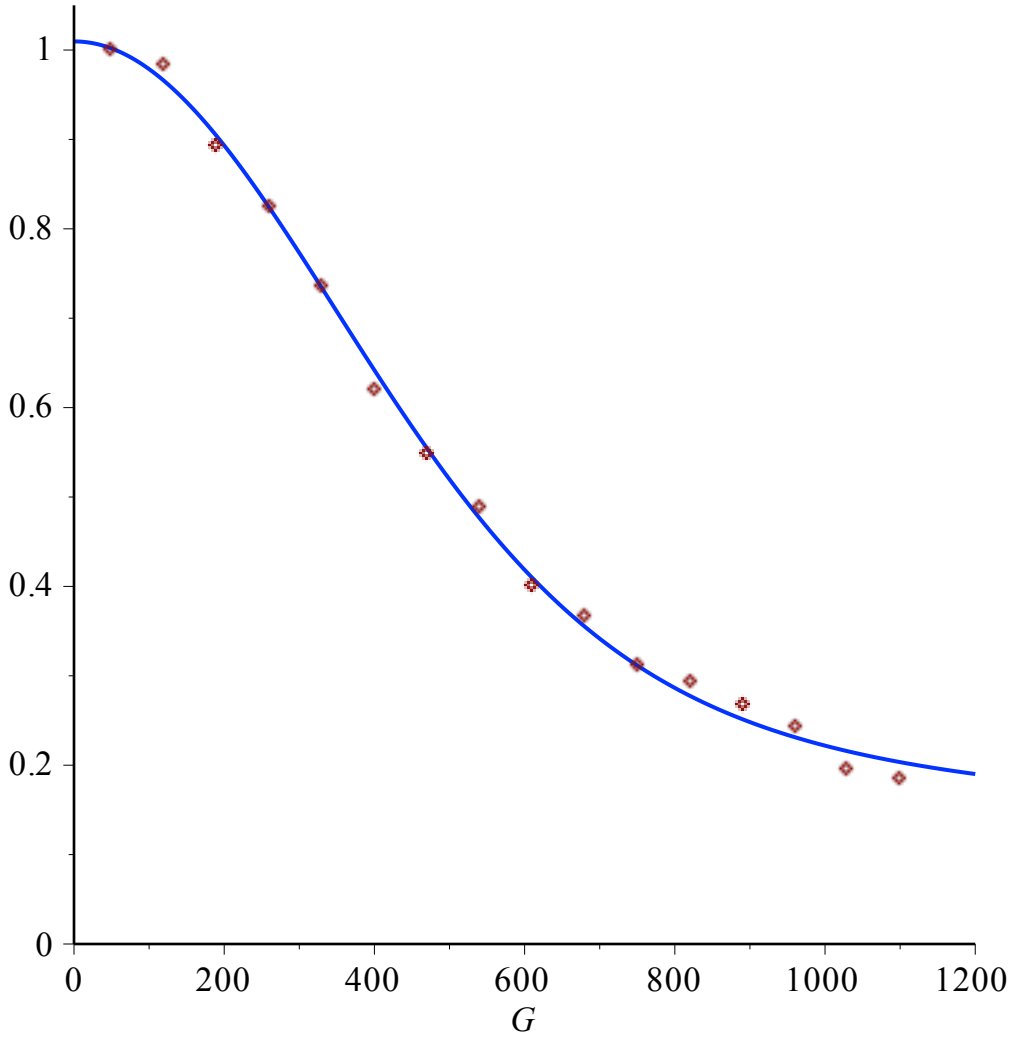
$a := Plot2D\left(Ab\left(rhs\left(\left(Solutionc_2\right)_1\right), rhs\left(\left(Solutionc_2\right)_2\right), G, rhs\left(\left(Solutionc_2\right)_3\right), rhs\left(\left(Solutionc_2\right)_4\right)\right), G = 0..1200, color = blue\right);$

$b := Plot2D(Gi, Ai, style = point, view = 0..1.05);$

$display(\{a, b\});$

$PLOT(...)$

$PLOT(...)$



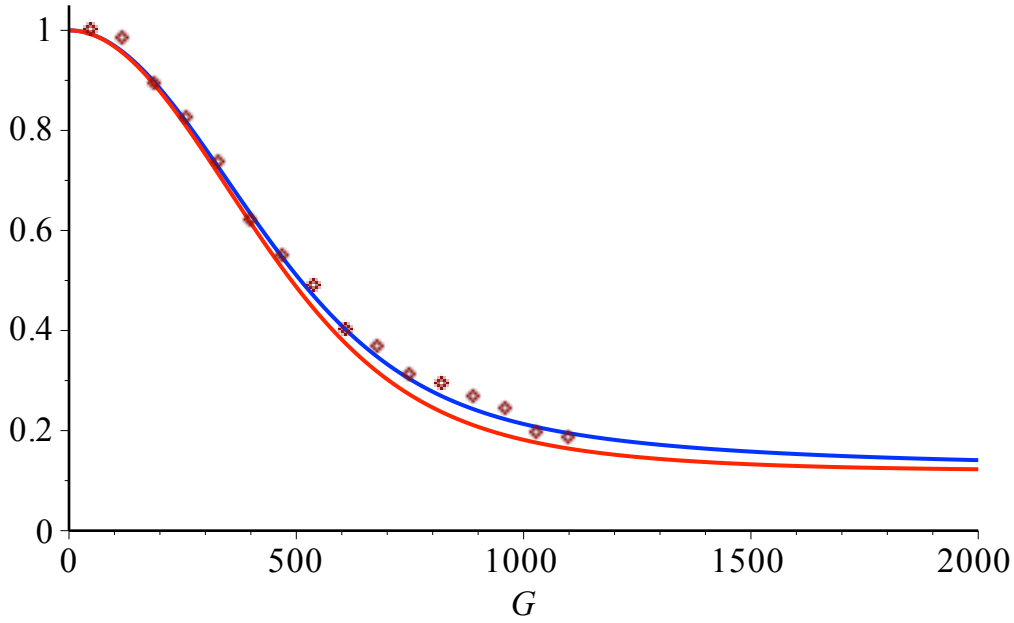

```
a := Plot2D(evalf(Ab(0.0, 0.3042, G, 0.88, 0.12)), G = 0..2000, color = blue);
b := Plot2D(evalf(Ab(0.03042, 0.3042, G, 0.88, 0.12)), G = 0..2000, color = red, view = 0..1.05);
#b := Plot2D(evalf(Ab(0.003042, 0.3042, G, 0.88, 0.12)), G = 0..2000, color
     = "Niagara DarkOrchid", view = 0..1.05);
 #b := Plot2D(evalf(Ab(0.2066, 0.2066, G, 0.8, 0.2)), G = 0..2000, color = red, view = 0..1.05);
#c := Plot2D(evalf(Ab(0.003682, 0.3682, G, 1, 0)), G = 0..1100, color = blue, linestyle = dash, view
     = 0..1.05);
 c := Plot2D(Gi, Ai, style = point, view = 0..1.05);

display({a, b, c});
```

PLOT(...)

PLOT(...)

PLOT(...)



$Solutionc := Minimize(ChiSquareb(Dpar, Dort, I0, 0), Dpar = 0..1.0, Dort = 0..1.0, I0 = 0.5..1.5,$
$initialpoint = \{Dpar = 0.0, Dort = 0.3, I0 = 1.0\}, variables = [Dpar, Dort, I0]);$

$[0.0209955902316021278, [Dpar = 0., Dort = 0.200658140394143, I0 = 0.972879109770371]]$ **(6)**

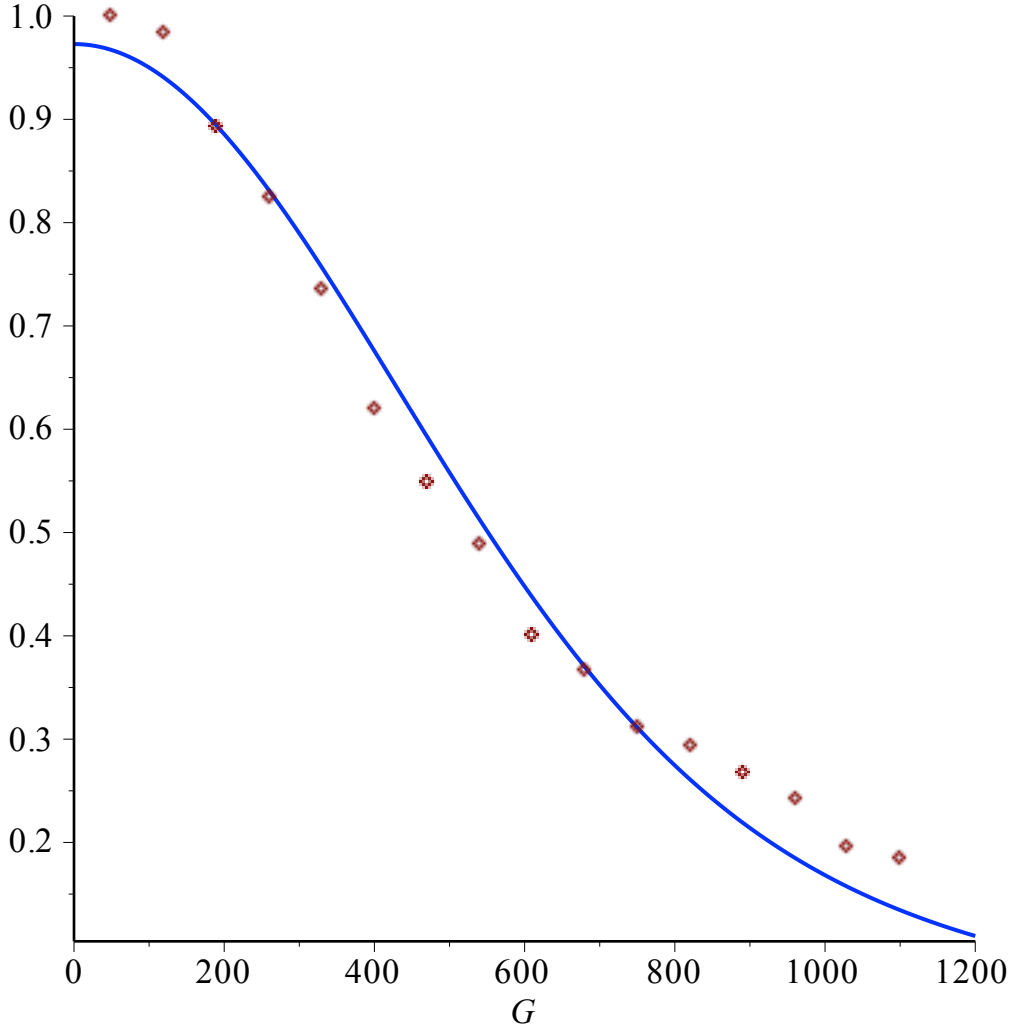
$a := Plot2D\left(Ab\left(rhs\left(\left(Solutionc_2\right)_1\right), rhs\left(\left(Solutionc_2\right)_2\right), G, rhs\left(\left(Solutionc_2\right)_3\right), 0\right), G = 0..1200,$
$color = blue\right);$

$b := Plot2D(Gi, Ai, style = point);$

$display(\{a, b\});$

$PLOT(...)$

$PLOT(...)$




```
Di := Vector([1.438e-10, 1.522e-10, 1.770e-10, 1.779e-10, 2.457e-10, 2.079e-10,
    2.638e-10, 2.587e-10, 3.042e-10, 3.195e-10, 3.433e-10, 3.682e-10], datatype = float);
Ti := Vector([534, 560, 587, 612, 637, 637, 662, 680, 704, 728, 751, 774], datatype = float);
Tleg := Vector([250, 300, 350, 400, 450, 500, 550], datatype = float);
Yleg := Vector([23, 23, 23, 23, 23, 23, 23], datatype = float);
Y := map(-ln, Di);
Myf := x -> 1000/x;
Myg := x -> 1/(8.314·x);
Myfleg := x -> 1000/(x + 273);
X := map(Myf, Ti);
Xtrue := map(Myg, Ti);
Xleg := map(Myfleg, Tleg);
LinearFit([1, x], Xtrue, Y, x, confidencelevel = 0.99, output = solutionmodule);
%:-Results( );
LinearFit([1, x], X, Y, x);
a := Plot2D(%, x = min(X) - 0.15 ..max(X) + 0.15, color = red);
```

```
b := Plot2D(X, Y, style = point, color = blue);
c := Plot2D(Xleg, Yleg, style = point, color = black);
display({a, b, c});
```

$$\begin{bmatrix} 1 \,..\, 12\ Vector_{column} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$

$$\begin{bmatrix} 1 \,..\, 12\ Vector_{column} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$

$$\begin{bmatrix} 250. \\ 300. \\ 350. \\ 400. \\ 450. \\ 500. \\ 550. \end{bmatrix}$$

$$\begin{bmatrix} 23. \\ 23. \\ 23. \\ 23. \\ 23. \\ 23. \\ 23. \end{bmatrix}$$

$$\begin{bmatrix} 1 \,..\, 12\ Vector_{column} \\ Data\ Type: anything \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$

$$x \rightarrow \frac{1000}{x}$$

$$x \rightarrow \frac{1}{8.314\,x}$$

$$x \rightarrow \frac{1000}{x + 273}$$

$$\begin{bmatrix} 1 \text{ .. } 12\ Vector_{column} \\ Data\ Type: anything \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$

$$\begin{bmatrix} 1 \text{ .. } 12\ Vector_{column} \\ Data\ Type: anything \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}$$

$$\begin{bmatrix} 1.91204588910134 \\ 1.74520069808028 \\ 1.60513643659711 \\ 1.48588410104012 \\ 1.38312586445367 \\ 1.29366106080207 \\ 1.21506682867558 \end{bmatrix}$$

module( ) **export** *Results*, *Settings*; **end module**

$$\begin{bmatrix} \text{"residualmeansquare"} = 0.00418546656300916, \text{"residualsumofsquares"} \end{bmatrix}$$

$$= 0.0418546656300916, \text{"residualstandarddeviation"} = 0.0646951819149553,$$

$$\text{"degreesoffreedom"} = 10, \text{"parametervalues"} = \begin{bmatrix} 19.4814500282904 \\ 14461.9748729811 \end{bmatrix}, \text{"parametervector"}$$

$$= \begin{bmatrix} 19.4814500282904 \\ 14461.9748729811 \end{bmatrix}, \text{"leastsquaresfunction"} = 19.4814500282904$$

$$+ 14461.9748729811\, x, \text{"standarderrors"} = \begin{bmatrix} 0.167405707536620 & 895.493401709056 \end{bmatrix},$$

$$\text{"confidenceintervals"} = \begin{bmatrix} 18.9508961873866 \,..20.0120038691943 \\ 11623.9147448526 \,..17300.0350011096 \end{bmatrix}, \text{"residuals"}$$

$$= \begin{bmatrix} 1 \,..\, 12\ Vector_{row} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}, \text{"leverages"} = \begin{bmatrix} 1 \,..\, 12\ Vector_{row} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix},$$

$$\text{"variancecovariancematrix"} = \begin{bmatrix} 0.0280246709158362 & -148.974907891680 \\ -148.974907891680 & 8.01908432504456\ 10^5 \end{bmatrix},$$

$$\text{"internallystandardizedresiduals"} = \begin{bmatrix} 1 \,..\, 12\ Vector_{column} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix},$$

$$\text{"externallystandardizedresiduals"} = \begin{bmatrix} 1 \,..\, 12\ Vector_{column} \\ Data\ Type: float_8 \\ Storage: rectangular \\ Order: Fortran\_order \end{bmatrix}, \text{"CookDstatistic"}$$

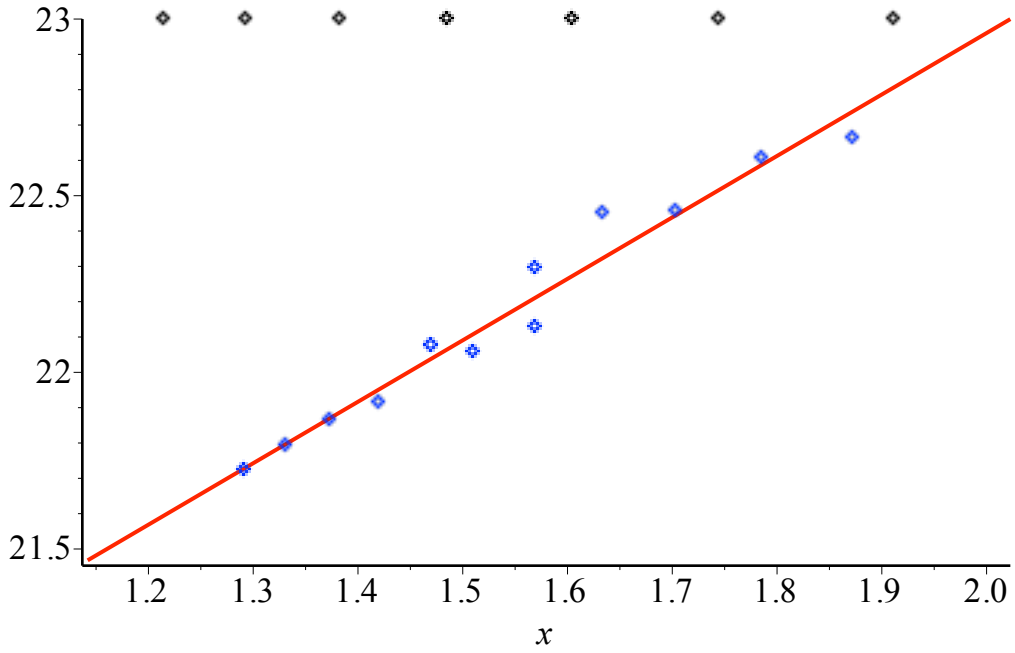
$$= \left[\begin{array}{l} 1 \,..\, 12\ Vector_{column} \\ Data\ Type:\ float_8 \\ Storage:\ rectangular \\ Order:\ Fortran\_order \end{array} \right], \text{"AtkinsonTstatistic"} = \left[\begin{array}{l} 1 \,..\, 12\ Vector_{column} \\ Data\ Type:\ float_8 \\ Storage:\ rectangular \\ Order:\ Fortran\_order \end{array} \right]$$

$$19.4814500282904 + 1.73947256124490\, x$$

$$PLOT(\ldots)$$

$$PLOT(\ldots)$$

$$PLOT(\ldots)$$



$$\frac{14461.9748729811}{6.02e23 \cdot 1.6e-19};$$

$$0.1501450879 \qquad \textbf{(7)}$$

$$\frac{895.493401709056}{6.02e23 \cdot 1.6e-19};$$

$$0.009297066048 \qquad \textbf{(8)}$$