

Instrumental Deviations from the Beer-Lambert Law

Measurement wavelength	Spectral bandpass	Absorber width	Maximum Absorptivity	Absorption Path length	Unabsorbed stray light
300	20	100	2	1	=0.0001*A23

Click the arrows above to change the values

Concentration	Measured absorbance
0.01	=Sheet2.E46
0.2	=Sheet2.F46
0.5	=Sheet2.G46
0.7	=Sheet2.H46
1	=Sheet2.I46
1.2	=Sheet2.J46
1.4	=Sheet2.K46
1.6	=Sheet2.L46
1.8	=Sheet2.M46
2	=Sheet2.N46

Blue text indicates user input cells.

1

Absorption peak shape

Gaussian

Lorentzian

σ of errors =STDEV(Sheet2.E50:N50)

Named variables

W	Wavelength
amax	Maximum absorptivity
aw	Absorber width (half-width of the absorption band)
b	Absorption path length
Izero	Incident intensity
sl	Stray light (fraction of incident light)
sw	Source width (spectral bandpass of monochromator)
slope	Slope of straight-line least squares fit to calibration curve
intercept	Intercept of straight-line least squares fit to calibration curve

© T. C. O'Haver, August 2, 2008

Wavelength		Inst. function
200	=1-200*ABS((A3-W)/(100))/(2*sw)	=IF(B3<0;0;B3)
=A3+5	=1-200*ABS((A4-W)/(100))/(2*sw)	=IF(B4<0;0;B4)
=A4+5	=1-200*ABS((A5-W)/(100))/(2*sw)	=IF(B5<0;0;B5)
=A5+5	=1-200*ABS((A6-W)/(100))/(2*sw)	=IF(B6<0;0;B6)
=A6+5	=1-200*ABS((A7-W)/(100))/(2*sw)	=IF(B7<0;0;B7)
=A7+5	=1-200*ABS((A8-W)/(100))/(2*sw)	=IF(B8<0;0;B8)
=A8+5	=1-200*ABS((A9-W)/(100))/(2*sw)	=IF(B9<0;0;B9)
=A9+5	=1-200*ABS((A10-W)/(100))/(2*sw)	=IF(B10<0;0;B10)
=A10+5	=1-200*ABS((A11-W)/(100))/(2*sw)	=IF(B11<0;0;B11)
=A11+5	=1-200*ABS((A12-W)/(100))/(2*sw)	=IF(B12<0;0;B12)
=A12+5	=1-200*ABS((A13-W)/(100))/(2*sw)	=IF(B13<0;0;B13)
=A13+5	=1-200*ABS((A14-W)/(100))/(2*sw)	=IF(B14<0;0;B14)
=A14+5	=1-200*ABS((A15-W)/(100))/(2*sw)	=IF(B15<0;0;B15)
=A15+5	=1-200*ABS((A16-W)/(100))/(2*sw)	=IF(B16<0;0;B16)
=A16+5	=1-200*ABS((A17-W)/(100))/(2*sw)	=IF(B17<0;0;B17)
=A17+5	=1-200*ABS((A18-W)/(100))/(2*sw)	=IF(B18<0;0;B18)
=A18+5	=1-200*ABS((A19-W)/(100))/(2*sw)	=IF(B19<0;0;B19)
=A19+5	=1-200*ABS((A20-W)/(100))/(2*sw)	=IF(B20<0;0;B20)
=A20+5	=1-200*ABS((A21-W)/(100))/(2*sw)	=IF(B21<0;0;B21)
=A21+5	=1-200*ABS((A22-W)/(100))/(2*sw)	=IF(B22<0;0;B22)
=A22+5	=1-200*ABS((A23-W)/(100))/(2*sw)	=IF(B23<0;0;B23)
=A23+5	=1-200*ABS((A24-W)/(100))/(2*sw)	=IF(B24<0;0;B24)
=A24+5	=1-200*ABS((A25-W)/(100))/(2*sw)	=IF(B25<0;0;B25)
=A25+5	=1-200*ABS((A26-W)/(100))/(2*sw)	=IF(B26<0;0;B26)
=A26+5	=1-200*ABS((A27-W)/(100))/(2*sw)	=IF(B27<0;0;B27)
=A27+5	=1-200*ABS((A28-W)/(100))/(2*sw)	=IF(B28<0;0;B28)
=A28+5	=1-200*ABS((A29-W)/(100))/(2*sw)	=IF(B29<0;0;B29)
=A29+5	=1-200*ABS((A30-W)/(100))/(2*sw)	=IF(B30<0;0;B30)
=A30+5	=1-200*ABS((A31-W)/(100))/(2*sw)	=IF(B31<0;0;B31)
=A31+5	=1-200*ABS((A32-W)/(100))/(2*sw)	=IF(B32<0;0;B32)
=A32+5	=1-200*ABS((A33-W)/(100))/(2*sw)	=IF(B33<0;0;B33)
=A33+5	=1-200*ABS((A34-W)/(100))/(2*sw)	=IF(B34<0;0;B34)
=A34+5	=1-200*ABS((A35-W)/(100))/(2*sw)	=IF(B35<0;0;B35)
=A35+5	=1-200*ABS((A36-W)/(100))/(2*sw)	=IF(B36<0;0;B36)
=A36+5	=1-200*ABS((A37-W)/(100))/(2*sw)	=IF(B37<0;0;B37)

=A37+5 =1-200*ABS((A38-W)/(100))/(2*sw)
 =A38+5 =1-200*ABS((A39-W)/(100))/(2*sw)
 =A39+5 =1-200*ABS((A40-W)/(100))/(2*sw)
 =A40+5 =1-200*ABS((A41-W)/(100))/(2*sw)
 =A41+5 =1-200*ABS((A42-W)/(100))/(2*sw)
 =A42+5 =1-200*ABS((A43-W)/(100))/(2*sw)

=IF(B38<0;0;B38)
 =IF(B39<0;0;B39)
 =IF(B40<0;0;B40)
 =IF(B41<0;0;B41)
 =IF(B42<0;0;B42)
 =IF(B43<0;0;B43)

lzero

Total intensity

=SUM(C3:C43)+sl*SUM(C3:C43)

Measured absorbance (y)

Theoretical absorbance

=IF(PeakShape="2";amax*(1/(1+((A38-300)/(0.5*aw))^2))+amax*(1/(1+((A38-150)/(0.5*aw))^2));amax*EXP(-1*((A38-300)/(0.6006*aw))^2)+amax*EXP(-1*((A38-150)/(0.6006*aw))^2))
 =IF(PeakShape="2";amax*(1/(1+((A39-300)/(0.5*aw))^2))+amax*(1/(1+((A39-150)/(0.5*aw))^2));amax*EXP(-1*((A39-300)/(0.6006*aw))^2)+amax*EXP(-1*((A39-150)/(0.6006*aw))^2))
 =IF(PeakShape="2";amax*(1/(1+((A40-300)/(0.5*aw))^2))+amax*(1/(1+((A40-150)/(0.5*aw))^2));amax*EXP(-1*((A40-300)/(0.6006*aw))^2)+amax*EXP(-1*((A40-150)/(0.6006*aw))^2))
 =IF(PeakShape="2";amax*(1/(1+((A41-300)/(0.5*aw))^2))+amax*(1/(1+((A41-150)/(0.5*aw))^2));amax*EXP(-1*((A41-300)/(0.6006*aw))^2)+amax*EXP(-1*((A41-150)/(0.6006*aw))^2))
 =IF(PeakShape="2";amax*(1/(1+((A42-300)/(0.5*aw))^2))+amax*(1/(1+((A42-150)/(0.5*aw))^2));amax*EXP(-1*((A42-300)/(0.6006*aw))^2)+amax*EXP(-1*((A42-150)/(0.6006*aw))^2))
 =IF(PeakShape="2";amax*(1/(1+((A43-300)/(0.5*aw))^2))+amax*(1/(1+((A43-150)/(0.5*aw))^2));amax*EXP(-1*((A43-300)/(0.6006*aw))^2)+amax*EXP(-1*((A43-150)/(0.6006*aw))^2))

Total transmitted intensity

Measured absorbance =

$amax*b*c=$

Predicted concentration =

Concentration error (real-predicted)

Concentration error as % of max concentration

Standard deviation of errors

Concentration

=Sheet1.H3	=Sheet1.H4	=Sheet1.H5	=Sheet1.H6	=Sheet1.H7	=Sheet1.H8	=Sheet1.H9
=C3*10^(-D3*b*E\$2)	=C3*10^(-D3*b*F\$2)	=C3*10^(-D3*b*G\$2)	###	###	###	###
=C4*10^(-D4*b*E\$2)	=C4*10^(-D4*b*F\$2)	=C4*10^(-D4*b*G\$2)	###	###	###	###
=C5*10^(-D5*b*E\$2)	=C5*10^(-D5*b*F\$2)	=C5*10^(-D5*b*G\$2)	###	###	###	###
=C6*10^(-D6*b*E\$2)	=C6*10^(-D6*b*F\$2)	=C6*10^(-D6*b*G\$2)	###	###	###	###
=C7*10^(-D7*b*E\$2)	=C7*10^(-D7*b*F\$2)	=C7*10^(-D7*b*G\$2)	###	###	###	###
=C8*10^(-D8*b*E\$2)	=C8*10^(-D8*b*F\$2)	=C8*10^(-D8*b*G\$2)	###	###	###	###
=C9*10^(-D9*b*E\$2)	=C9*10^(-D9*b*F\$2)	=C9*10^(-D9*b*G\$2)	###	###	###	###
=C10*10^(-D10*b*E\$2)	=C10*10^(-D10*b*F\$2)	=C10*10^(-D10*b*G\$2)	###	###	###	###
=C11*10^(-D11*b*E\$2)	=C11*10^(-D11*b*F\$2)	=C11*10^(-D11*b*G\$2)	###	###	###	###
=C12*10^(-D12*b*E\$2)	=C12*10^(-D12*b*F\$2)	=C12*10^(-D12*b*G\$2)	###	###	###	###
=C13*10^(-D13*b*E\$2)	=C13*10^(-D13*b*F\$2)	=C13*10^(-D13*b*G\$2)	###	###	###	###
=C14*10^(-D14*b*E\$2)	=C14*10^(-D14*b*F\$2)	=C14*10^(-D14*b*G\$2)	###	###	###	###
=C15*10^(-D15*b*E\$2)	=C15*10^(-D15*b*F\$2)	=C15*10^(-D15*b*G\$2)	###	###	###	###
=C16*10^(-D16*b*E\$2)	=C16*10^(-D16*b*F\$2)	=C16*10^(-D16*b*G\$2)	###	###	###	###
=C17*10^(-D17*b*E\$2)	=C17*10^(-D17*b*F\$2)	=C17*10^(-D17*b*G\$2)	###	###	###	###
=C18*10^(-D18*b*E\$2)	=C18*10^(-D18*b*F\$2)	=C18*10^(-D18*b*G\$2)	###	###	###	###
=C19*10^(-D19*b*E\$2)	=C19*10^(-D19*b*F\$2)	=C19*10^(-D19*b*G\$2)	###	###	###	###
=C20*10^(-D20*b*E\$2)	=C20*10^(-D20*b*F\$2)	=C20*10^(-D20*b*G\$2)	###	###	###	###
=C21*10^(-D21*b*E\$2)	=C21*10^(-D21*b*F\$2)	=C21*10^(-D21*b*G\$2)	###	###	###	###
=C22*10^(-D22*b*E\$2)	=C22*10^(-D22*b*F\$2)	=C22*10^(-D22*b*G\$2)	###	###	###	###
=C23*10^(-D23*b*E\$2)	=C23*10^(-D23*b*F\$2)	=C23*10^(-D23*b*G\$2)	###	###	###	###
=C24*10^(-D24*b*E\$2)	=C24*10^(-D24*b*F\$2)	=C24*10^(-D24*b*G\$2)	###	###	###	###
=C25*10^(-D25*b*E\$2)	=C25*10^(-D25*b*F\$2)	=C25*10^(-D25*b*G\$2)	###	###	###	###
=C26*10^(-D26*b*E\$2)	=C26*10^(-D26*b*F\$2)	=C26*10^(-D26*b*G\$2)	###	###	###	###
=C27*10^(-D27*b*E\$2)	=C27*10^(-D27*b*F\$2)	=C27*10^(-D27*b*G\$2)	###	###	###	###
=C28*10^(-D28*b*E\$2)	=C28*10^(-D28*b*F\$2)	=C28*10^(-D28*b*G\$2)	###	###	###	###
=C29*10^(-D29*b*E\$2)	=C29*10^(-D29*b*F\$2)	=C29*10^(-D29*b*G\$2)	###	###	###	###
=C30*10^(-D30*b*E\$2)	=C30*10^(-D30*b*F\$2)	=C30*10^(-D30*b*G\$2)	###	###	###	###
=C31*10^(-D31*b*E\$2)	=C31*10^(-D31*b*F\$2)	=C31*10^(-D31*b*G\$2)	###	###	###	###
=C32*10^(-D32*b*E\$2)	=C32*10^(-D32*b*F\$2)	=C32*10^(-D32*b*G\$2)	###	###	###	###
=C33*10^(-D33*b*E\$2)	=C33*10^(-D33*b*F\$2)	=C33*10^(-D33*b*G\$2)	###	###	###	###
=C34*10^(-D34*b*E\$2)	=C34*10^(-D34*b*F\$2)	=C34*10^(-D34*b*G\$2)	###	###	###	###
=C35*10^(-D35*b*E\$2)	=C35*10^(-D35*b*F\$2)	=C35*10^(-D35*b*G\$2)	###	###	###	###
=C36*10^(-D36*b*E\$2)	=C36*10^(-D36*b*F\$2)	=C36*10^(-D36*b*G\$2)	###	###	###	###
=C37*10^(-D37*b*E\$2)	=C37*10^(-D37*b*F\$2)	=C37*10^(-D37*b*G\$2)	###	###	###	###

=C38*10^(-D38*b*E\$2)	=C38*10^(-D38*b*F\$2)	=C38*10^(-D38*b*G\$2)	###	###	###	###
=C39*10^(-D39*b*E\$2)	=C39*10^(-D39*b*F\$2)	=C39*10^(-D39*b*G\$2)	###	###	###	###
=C40*10^(-D40*b*E\$2)	=C40*10^(-D40*b*F\$2)	=C40*10^(-D40*b*G\$2)	###	###	###	###
=C41*10^(-D41*b*E\$2)	=C41*10^(-D41*b*F\$2)	=C41*10^(-D41*b*G\$2)	###	###	###	###
=C42*10^(-D42*b*E\$2)	=C42*10^(-D42*b*F\$2)	=C42*10^(-D42*b*G\$2)	###	###	###	###
=C43*10^(-D43*b*E\$2)	=C43*10^(-D43*b*F\$2)	=C43*10^(-D43*b*G\$2)	###	###	###	###
=SUM(E3:E43)+sl*\$C\$45	###	=SUM(G3:G43)+sl*\$C\$45	###	###	###	###
=LOG(lzero/E45;10)	=LOG(lzero/F45;10)	=LOG(lzero/G45;10)	###	###	###	###
=E2*\$D\$23*b	=F2*\$D\$23*b	=G2*\$D\$23*b	=H2*\$D\$23*b	=I2*\$D\$23*b	=J2*\$D\$23*b	=K2*\$D\$23*b
=(E46-intercept)/slope	=(F46-intercept)/slope	=(G46-intercept)/slope	###	###	###	###
=E2-E48	=F2-F48	=G2-G48	=H2-H48	=I2-I48	=J2-J48	=K2-K48
=E49/\$N\$47	=F49/\$N\$47	=G49/\$N\$47	=H49/\$N\$47	=I49/\$N\$47	=J49/\$N\$47	=K49/\$N\$47
=STDEV(E50:N50)	slope=	=SLOPE(E\$46:N\$46;E\$2:N\$2)				
	Intercept=	=INTERCEPT(E\$46:N\$46;E\$2:N\$2)				
	R2=	=RSQ(E\$46:N\$46;E\$2:N\$2)				

