Appendix

Si hoc legere scis, nimis eruditonis habes

Concentration Variance of Self-Complexing Molecules

The plots obtained in Chapter 3—that show how changes in K_a values affect the distribution of monomers/oligomers in a solution of a self-complementary monomer over a given concentration range—were obtained using a spreadsheet written in Microsoft Excel 98. The model employed (shown in Figure 3.20) for these calculations (Page 105) assumes that no oligomers larger than trimers are formed. Therefore, the plots obtained are only approximations, but appear to fit the observed experimental data. The spreadsheet has the capacity to solve both reducible and irreducible cubic equations, and follows standard methods, as discussed in Rosenbach, J. B.; Whitman, E. A. *College Algebra, (Revised Edition)*; Ginn and Company: Boston, 1939, pp. 265–269. What follows are the cell entries: those containing *comments* are italicized, those requiring **input** are in bold, and those containing calculations and/or equalities appear in regular text.

A1 = *"Total Dissolved Monomer Concentration [M] in M"*
B1 = *"Log_{10}[M]"*
C1 = *"K_{a2} (M^{-1})"*
D1 = *"[a1] (M)"*
E1 = *"[a2] (M)"*
F1 = *"[a3] (M)"*
G1 = *"[c1] (M)"*
H1 = *"[c2] (M)"*
I1 = *"[c3] (M)"*
J1 = *"Total Concentration of Species in Solution"*
K1 = *"Total Dissolved Monomer Concentration [M] in M"*
L1 = *"%a1"*
M1 = *"%c1"*
N1 = *"%a2"*
O1 = *"%c2"*
P1 = *"%a3"*
Q1 = *"%c3"*
R1 = *"100%"*
A2 = 0.000001
B2 = LOG(A2)
C2 **Enter value of K_{a2} (M^{-1}) in here**
D2 = F51
E2 = C2*(F51^2)
F2 = C2*C4*(F51^3)
G2 = C6*F51
H2 = C8*C2*(F51^2)
I2 = C10*C4*C2*(F51^3)
J2 = I2+H2+G2+F2+E2+D2
K2 = (F51*(1+C6))+((F51^2)*((2*C2)+(2*C2*C8)))+((F51^3)*(3*C2*C4)+(3*C10*C4*C2)))
L2 = (D2/J2)*100
M2 = (G2/J2)*100
N2 = (E2/J2)*100
O2 = (H2/J2)*100
P2 = (F2/J2)*100
Q2 = (I2/J2)*100
R2 = L2+M2+N2+O2+P2+Q2
A3 = 0.00001
B3 = LOG(A3)
C3 = *"K_{a3} (M^{-1})"*
D3 = F87
E3 = C2*(F87^2)

F3 = C2*C4*(F87^3)
G3 = C6*F87
H3 = C8*C2*(F87^2)
I3 = C10*C4*C2*(F87^3)
J3 = I3+H3+G3+F3+E3+D3
K3 = (F87*(1+C6))+((F87^2)*((2*C2)+(2*C2*C8)))+((F87^3)*(3*C2*C4)+(3*C10*C4*C2)))
L3 = (D3/J3)*100
M3 = (G3/J3)*100
N3 = (E3/J3)*100
O3 = (H3/J3)*100
P3 = (F3/J3)*100
Q3 = (I3/J3)*100
R3 = L3+M3+N3+O3+P3+Q3
A4 = 0.0001
B4 = LOG(A4)
C4 **Enter value of K_{a3} (M^{-1}) in here**
D4 = F124
E4 = C2*(F124^2)
F4 = C2*C4*(F124^3)
G4 = C6*F124
H4 = C8*C2*(F124^2)
I4 = C10*C4*C2*(F124^3)
J4 = I4+H4+G4+F4+E4+D4
K4 = (F124*(1+C6))+((F124^2)*((2*C2)+(2*C2*C8)))+((F124^3)*(3*C2*C4)+(3*C10*C4*C2)))
L4 = (D4/J4)*100
M4 = (G4/J4)*100
N4 = (E4/J4)*100
O4 = (H4/J4)*100
P4 = (F4/J4)*100
Q4 = (I4/J4)*100
R4 = L4+M4+N4+O4+P4+Q4
A5 = 0.001
B5 = LOG(A5)
C5 = *"K_{c1}"*
D5 = F161
E5 = C2*(F161^2)
F5 = C2*C4*(F161^3)
G5 = C6*F161
H5 = C8*C2*(F161^2)
I5 = C10*C4*C2*(F161^3)
J5 = I5+H5+G5+F5+E5+D5
K5 = (F161*(1+C6))+((F161^2)*((2*C2)+(2*C2*C8)))+((F161^3)*(3*C2*C4)+(3*C10*C4*C2)))
L5 = (D5/J5)*100
M5 = (G5/J5)*100
N5 = (E5/J5)*100
O5 = (H5/J5)*100
P5 = (F5/J5)*100
Q5 = (I5/J5)*100
R5 = L5+M5+N5+O5+P5+Q5
A6 = 0.01
B6 = LOG(A6)
C6 **Enter value of K_{c1} (pure number) in here**
D6 = F197
E6 = C2*(F197^2)
F6 = C2*C4*(F197^3)
G6 = C6*F197
H6 = C8*C2*(F197^2)
I6 = C10*C4*C2*(F197^3)
J6 = I6+H6+G6+F6+E6+D6
K6 = (F197*(1+C6))+((F197^2)*((2*C2)+(2*C2*C8)))+((F197^3)*(3*C2*C4)+(3*C10*C4*C2)))
L6 = (D6/J6)*100

M6 = (G6/J6)*100
N6 = (E6/J6)*100
O6 = (H6/J6)*100
P6 = (F6/J6)*100
Q6 = (I6/J6)*100
R6 = L6+M6+N6+O6+P6+Q6
A7 = 0.1
B7 = LOG(A7)
C7 = *"K_{c2}"*
D7 = F234
E7 = C2*(F234^2)
F7 = C2*C4*(F234^3)
G7 = C6*F234
H7 = C8*C2*(F234^2)
I7 = C10*C4*C2*(F234^3)
J7 = I7+H7+G7+F7+E7+D7
K7 = (F234*(1+C6))+((F234^2)*((2*C2)+(2*C2*C8)))+((F234^3)*(3*C2*C4)+(3*C10*C4*C2)))
L7 = (D7/J7)*100
M7 = (G7/J7)*100
N7 = (E7/J7)*100
O7 = (H7/J7)*100
P7 = (F7/J7)*100
Q7 = (I7/J7)*100
R7 = L7+M7+N7+O7+P7+Q7
A8 = 1
B8 = LOG(A8)
C8 **Enter value of K_{c2} (pure number) in here**
D8 = F271
E8 = C2*(F271^2)
F8 = C2*C4*(F271^3)
G8 = C6*F271
H8 = C8*C2*(F271^2)
I8 = C10*C4*C2*(F271^3)
J8 = I8+H8+G8+F8+E8+D8
K8 = (F271*(1+C6))+((F271^2)*((2*C2)+(2*C2*C8)))+((F271^3)*(3*C2*C4)+(3*C10*C4*C2)))
L8 = (D8/J8)*100
M8 = (G8/J8)*100
N8 = (E8/J8)*100
O8 = (H8/J8)*100
P8 = (F8/J8)*100
Q8 = (I8/J8)*100
R8 = L8+M8+N8+O8+P8+Q8
A9 = 10
B9 = LOG(A9)
C9 = *"K_{c3}"*
D9 = F309
E9 = C2*(F309^2)
F9 = C2*C4*(F309^3)
G9 = C6*F309
H9 = C8*C2*(F309^2)
I9 = C10*C4*C2*(F309^3)
J9 = I9+H9+G9+F9+E9+D9
K9 = (F309*(1+C6))+((F309^2)*((2*C2)+(2*C2*C8)))+((F309^3)*(3*C2*C4)+(3*C10*C4*C2)))
L9 = (D9/J9)*100
M9 = (G9/J9)*100
N9 = (E9/J9)*100
O9 = (H9/J9)*100
P9 = (F9/J9)*100
Q9 = (I9/J9)*100
R9 = L9+M9+N9+O9+P9+Q9
A10 = 100

B10 = LOG(A10)
C10 Enter value of K_{c3} (pure number) in here
D10 = F346
E10 = C2*(F346^2)
F10 = C2*C4*(F346^3)
G10 = C6*F346
H10 = C8*C2*(F346^2)
I10 = C10*C4*C2*(F346^3)
J10 = I10+H10+G10+F10+E10+D10
K10 = (F346*(1+C6))+((F346^2)*((2*C2)+(2*C2*C8)))+((F346^3)*(3*C2*C4)+(3*C10*C4*C2)))
L10 = (D10/J10)*100
M10 = (G10/J10)*100
N10 = (E10/J10)*100
O10 = (H10/J10)*100
P10 = (F10/J10)*100
Q10 = (I10/J10)*100
R10 = L10+M10+N10+O10+P10+Q10
A11 Enter a specific value of [*M*] (M) in here to determine the resulting solution composition
B11 = LOG(A11)
D11 = F382
E11 = C2*(F382^2)
F11 = C2*C4*(F382^3)
G11 = C6*F382
H11 = C8*C2*(F382^2)
I11 = C10*C4*C2*(F382^3)
J11 = I11+H11+G11+F11+E11+D11
K11 = (F382*(1+C6))+((F382^2)*((2*C2)+(2*C2*C8)))+((F382^3)*(3*C2*C4)+(3*C10*C4*C2)))
L11 = (D11/J11)*100
M11 = (G11/J11)*100
N11 = (E11/J11)*100
O11 = (H11/J11)*100
P11 = (F11/J11)*100
Q11 = (I11/J11)*100
R11 = L11+M11+N11+O11+P11+Q11
B16 = "Coefficient of x^3"
C16 = "Coefficient of x^2"
D16 = "Coefficient of x"
B17 = (3*C2*C4)+(3*C10*C4*C2)
C17 = (2*C2)+(2*C2*C8)
D17 = (1+C6)

The following section solves the cubic equation for $[M] = 10^{-6}$ M

B25 = "Normalized coefficient of x^3"
C25 = "Normalized coefficient of x^2"
D25 = "Normalized coefficient of x"
E25 = "Normalized constant"

The coefficient of the x^3 term must be 1 in order to solve the equation. The 'normalized' values in the four cells above are obtained by dividing the cubic equation by the coefficient of x^3.

H25 = "p"
I25 = "q"
J25 = "R"
B26 = 1
C26 = C17/B17
D26 = D17/B17
E26 = -A2/B17
H26 = D26-((C26^2)/3)
I26 = E26-((C26*D26)/3)+((2/27)*C26^3))
J26 = ((1/27)*(H26^3))+(0.25*I26*I26)

K26 = SIGN(J26)+1
L26 = SIGN(K26)
M26 = ABS(L26-1)
I27 = -0.5*I26
J27 = SIGN(J26)*J26
J28 = SQRT(J27)
J29 = -1*J28
H30 = *"u^3 (A)"*
I30 = *"v^3 (B)"*
H31 = COMPLEX(I27,J28)
I31 = COMPLEX(I27,J29)
H32 = IMPOWER((H31,1/3)
I32 = IMPOWER(I31,1/3)
H33 = I27+J28
I33 = I27-J28
M34 = SIGN(H26)+1
N34 = SIGN(M34)
O34 = ABS(N34-1)
H35 = *"$\sqrt[3]{A}$"*
I35 = *"$\sqrt[3]{B}$"*
H36 = H33^(1/3)
I36 = I33^(1/3)
O36 = (2*O34)-1
M38 = A48*M26
F39 = *"If R is positive"*
G39 = *"If R is negative"*
M39 = M38+L26
A40 = *"w"*
B40 = *"w^2"*
E40 = *"1st Root"*
F40 = (H33^(1/3))+(I33^(1/3))-(C26/3)
G40 = B58
A41 = COMPLEX(-0.5,A43)
B41 = COMPLEX(-0.5,A44)
E41 = *"2nd Root"*
F41 = IMSUM((IMPRODUCT(A41,H36)),(IMPRODUCT(B41,I36)),(C26/-3))
G41 = C58
E42 = *"3rd Root"*
F42 = IMSUM((IMPRODUCT(B41,H36)),(IMPRODUCT(A41,I36)),(C26/-3))
G42 = D58
A43 = SQRT(3)/2
M43 = I26*M26
A44 = -A43
M44 = M43+L26
A47 = *"r"*
A48 = SQRT((-1/27)*(H26^3)*O36)
A49 = *"cos θ"*
B49 = *"θ"*
C49 = *"π"*
A50 = ((-0.5*M44)/M39)
B50 = (ACOS(A50))/((PI())*2)*360
C50 = PI()
F50 = *"Roots"*
F51 = IMSUM((IMPRODUCT(F40,L26)),(IMPRODUCT(G40,M26)))
B52 = *"θ / 3"*
F52 = IMSUM((IMPRODUCT(F41,L26)),(IMPRODUCT(G41,M26)))
B53 = B50/3
F53 = IMSUM((IMPRODUCT(F42,L26)),(IMPRODUCT(G42,M26)))
B55 = *"cos θ / 3"*
C55 = *"cos (θ + 360)/3"*
D55 = *"cos (θ + 720)/3"*

B56 = COS((B53/360)*(2*C50))
C56 = (2*(M39^(1/3))*COS((((B50+360)/3)/360)*2*C50))-(C26/3)
D56 = (2*(M39^(1/3))*COS((((B50+720)/3)/360)*2*C50))-(C26/3)
B58 = (2*(M39^(1/3))*B56)-(C26/3)
C58 = C56
D58 = D56

The following section solves the cubic equation for $[M] = 10^{-5}$ M

B61 = *"Normalized coefficient of x^3"*
C61 = *"Normalized coefficient of x^2"*
D61 = *"Normalized coefficient of x"*
E61 = *"Normalized constant"*
H61 = *"p"*
I61 = *"q"*
J61 = *"R"*
B62 = 1
C62 = C17/B17
D62 = D17/B17
E62 = -A3/B17
H62 = D62-((C62^2)/3)
I62 = E62-((C62*D62)/3)+((2/27)*C62^3))
J62 = ((1/27)*(H62^3))+(0.25*I62*I62)
K62 = SIGN(J62)+1
L62 = SIGN(K62)
M62 = ABS(L62-1)
I63 = -0.5*I62
J63 = SIGN(J62)*J62
J64 = SQRT(J63)
J65 = -1*J64
H66 = *"u^3 (A)"*
I66 = *"v^3 (B)"*
H67 = COMPLEX(I63,J64)
I67 = COMPLEX(I63,J65)
H68 = IMPOWER((H67,1/3)
I68 = IMPOWER(I67,1/3)
H69 = I63+J64
I69 = I63-J64
M70 = SIGN(H62)+1
N70 = SIGN(M70)
O70 = ABS(N70-1)
H71 = *"$\sqrt[3]{A}$"*
I71 = *"$\sqrt[3]{B}$"*
H72 = H69^(1/3)
I72 = I69^(1/3)
O72 = (2*O70)-1
M74 = A84*M62
F75 = *"If R is positive"*
G75 = *"If R is negative"*
M75 = M74+L62
A76 = *"w"*
B76 = *"w^2"*
E76 = *"1st Root"*
F76 = (H69^(1/3))+(I69^(1/3))-(C62/3)
G76 = B94
A77 = COMPLEX(-0.5,A79)
B77 = COMPLEX(-0.5,A80)
E77 = *"2nd Root"*
F77 = IMSUM((IMPRODUCT(A77,H72)),(IMPRODUCT(B77,I72)),(C62/-3))
G77 = C94

E78 = *"3rd Root"*
F78 = IMSUM((IMPRODUCT(B77,H72)),(IMPRODUCT(A77,I72)),(C62/-3))
G78 = D94
A79 = SQRT(3)/2
M79 = I62*M62
A80 = -A79
M80 = M79+L62
A83 = *"r"*
A84 = SQRT((-1/27)*(H62^3)*O72)
A85 = *"cos θ"*
B85 = *"θ"*
C85 = *"π"*
A86 = ((-0.5*M80)/M75)
B86 = (ACOS(A86))/((PI())*2)*360
C86 = PI()
F86 = *"Roots"*
F87 = IMSUM((IMPRODUCT(F76,L62)),(IMPRODUCT(G76,M62)))
B88 = *"θ / 3"*
F88 = IMSUM((IMPRODUCT(F77,L62)),(IMPRODUCT(G77,M62)))
B89 = B86/3
F89 = IMSUM((IMPRODUCT(F78,L62)),(IMPRODUCT(G78,M62)))
B91 = *"cos θ / 3"*
C91 = *"cos (θ + 360)/3"*
D91 = *"cos (θ + 720)/3"*
B92 = COS((B89/360)*(2*C86))
C92 = (2*(M75^(1/3))*COS((((B86+360)/3)/360)*2*C86))-(C62/3)
D92 = (2*(M75^(1/3))*COS((((B86+720)/3)/360)*2*C86))-(C62/3)
B94 = 2*(M75^(1/3))*B92)-(C62/3)
C94 = C92
D94 = D92

The following section solves the cubic equation for $[M] = 10^{-4}$ M

B98 = *"Normalized coefficient of x^3"*
C98 = *"Normalized coefficient of x^2"*
D98 = *"Normalized coefficient of x"*
E98 = *"Normalized constant"*
H98 = *"p"*
I98 = *"q"*
J98 = *"R"*
B99 = 1
C99 = C17/B17
D99 = D17/B17
E99 = -A4/B17
H99 = D99-((C99^2)/3)
I99 = E99-((C99*D99)/3)+((2/27)*C99^3))
J99 = ((1/27)*(H99^3))+(0.25*I99*I99)
K99 = SIGN(J99)+1
L99 = SIGN(K99)
M99 = ABS(L99-1)
I100 = -0.5*I99
J100 = SIGN(J99)*J99
J101 = SQRT(J100)
J102 = -1*J101
H103 = *"u^3 (A)"*
I103 = *"v^3 (B)"*
H104 = COMPLEX(I100,J101)
I104 = COMPLEX(I100,J102)
H105 = IMPOWER((H104,1/3)
I105 = IMPOWER(I104,1/3)
H106 = I100+J101

I106 = I100-J101
M107 = SIGN(H99)+1
N107 = SIGN(M107)
O107 = ABS(N107-1)
H108 = *"$\sqrt[3]{A}$"*
I108 = *"$\sqrt[3]{B}$"*
H109 = H106^(1/3)
I109 = I106^(1/3)
O109 = (2*O107)-1
M111 = A121*M99
F112 = *"If R is positive"*
G112 = *"If R is negative"*
M112 = M111+L99
A113 = *"w"*
B113 = *"w^2"*
E113 = *"1st Root"*
F113 = (H106^(1/3))+(I106^(1/3))-(C99/3)
G113 = B131
A114 = COMPLEX(-0.5,A116)
B114 = COMPLEX(-0.5,A117)
E114 = *"2nd Root"*
F114 = IMSUM((IMPRODUCT(A114,H109)),(IMPRODUCT(B114,I109)),(C99/-3))
G114 = C131
E115 = *"3rd Root"*
F115 = IMSUM((IMPRODUCT(B114,H109)),(IMPRODUCT(A114,I109)),(C99/-3))
G115 = D131
A116 = SQRT(3)/2
M116 = I99*M99
A117 = -A116
M117 = M116+L99
A120 = *"r"*
A121 = SQRT((-1/27)*(H99^3)*O109)
A122 = *"cos θ"*
B122 = *"θ"*
C122 = *"π"*
A123 = ((-0.5*M117)/M112)
B123 = (ACOS(A123))/((PI())*2)*360
C123 = PI()
F123 = *"Roots"*
F124 = IMSUM((IMPRODUCT(F113,L99)),(IMPRODUCT(G113,M99)))
B125 = "θ / 3"
F125 = IMSUM((IMPRODUCT(F114,L99)),(IMPRODUCT(G114,M99)))
B126 = *B123/3*
F126 = IMSUM((IMPRODUCT(F115,L99)),(IMPRODUCT(G115,M99)))
B128 = *"cos θ / 3"*
C128 = *"cos (θ + 360)/3"*
D128 = *"cos (θ + 720)/3"*
B129 = COS((B126/360)*(2*C123))
C129 = (2*(M112^(1/3))*COS((((B123+360)/3)/360)*2*C123))-(C99/3)
D129 = (2*(M112^(1/3))*COS((((B123+720)/3)/360)*2*C123))-(C99/3)
B131 = (2*(M112^(1/3))*B129)-(C99/3)
C131 = C129
D131 = D129

The following section solves the cubic equation for $[M] = 10^{-3}$ M

B135 = *"Normalized coefficient of x^3"*
C135 = *"Normalized coefficient of x^2"*
D135 = *"Normalized coefficient of x"*
E135 = *"Normalized constant"*
H135 = *"p"*

I135 = *"q"*
J135 = *"R"*
B136 = 1
C136 = C17/B17
D136 = D17/B17
E136 = -A5/B17
H136 = D136-((C136^2)/3)
I136 = E136-((C136*D136)/3)+((2/27)*C136^3))
J136 = ((1/27)*(H136^3))+(0.25*I136*I136)
K136 = SIGN(J136)+1
L136 = SIGN(K136)
M136 = ABS(L136-1)
I137 = -0.5*I136
J137 = SIGN(J136)*J136
J138 = SQRT(J137)
J139 = -1*J138
H140 = *"u^3 (A)"*
I140 = *"v^3 (B)"*
H141 = COMPLEX(I137,J138)
I141 = COMPLEX(I137,J139)
H142 = IMPOWER((H141,1/3)
I142 = IMPOWER(I141,1/3)
H143 = I137+J138
I143 = I137-J138
M144 = SIGN(H136)+1
N144 = SIGN(M144)
O144 = ABS(N144-1)
H145 = *"$\sqrt[3]{A}$"*
I145 = *"$\sqrt[3]{B}$"*
H146 = H143^(1/3)
I146 = I143^(1/3)
O146 = (2*O144)-1
M148 = A158*M136
F149 = *"If R is positive"*
G149 = *"If R is negative"*
M149 = M148+L126
A150 = *"w"*
B150 = *"w^2"*
E150 = *"1st Root"*
F150 = (H143^(1/3))+(I143^(1/3))-(C136/3)
G150 = B168
A151 = COMPLEX(-0.5,A153)
B151 = COMPLEX(-0.5,A154)
E151 = *"2nd Root"*
F151 = IMSUM((IMPRODUCT(A151,H146)),(IMPRODUCT(B151,I146)),(C136/-3))
G151 = C168
E152 = *"3rd Root"*
F152 = IMSUM((IMPRODUCT(B151,H146)),(IMPRODUCT(A151,I146)),(C136/-3))
G152 = D168
A153 = SQRT(3)/2
M153 = I136*M136
A154 = -A153
M154 = M153+L136
A157 = *"r"*
A158 = SQRT((-1/27)*(H136^3)*O146)
A159 = *"cos θ"*
B159 = *"θ"*
C159 = *"π"*
A160 = ((-0.5*M154)/M149)
B160 = (ACOS(A160))/((PI())*2)*360
C160 = PI()

F160 = *"Roots"*
F161 = IMSUM((IMPRODUCT(F150,L136)),(IMPRODUCT(G150,M136)))
B162 = *"θ / 3"*
F162 = IMSUM((IMPRODUCT(F151,L136)),(IMPRODUCT(G151,M136)))
B163 = B160/3
F163 = IMSUM((IMPRODUCT(F152,L136)),(IMPRODUCT(G152,M136)))
B165 = *"cos θ / 3"*
C165 = *"cos (θ + 360)/3"*
D165 = *"cos (θ + 720)/3"*
B166 = COS((B163/360)*(2*C160))
C166 = (2*(M149^(1/3))*COS((((B160+360)/3)/360)*2*C160))-(C136/3)
D166 = (2*(M149^(1/3))*COS((((B160+720)/3)/360)*2*C160))-(C136/3)
B168 = (2*(M149^(1/3))*B166)-(C136/3)
C168 = C166
D168 = D166

The following section solves the cubic equation for $[M] = 10^{-2}$ M

B171 = *"Normalized coefficient of x^3"*
C171 = *"Normalized coefficient of x^2"*
D171 = *"Normalized coefficient of x"*
E171 = *"Normalized constant"*
H171 = *"p"*
I171 = *"q"*
J171 = *"R"*
B172 = 1
C172 = C17/B17
D172 = D17/B17
E172 = -A6/B17
H172 = D172-((C172^2)/3)
I172 = E172-((C172*D172)/3)+((2/27)*C172^3))
J172 = ((1/27)*(H172^3))+(0.25*I172*I172)
K172 = SIGN(J172)+1
L172 = SIGN(K172)
M172 = ABS(L172-1)
I173 = -0.5*I172
J173 = SIGN(J172)*J172
J174 = SQRT(J173)
J175 = -1*J174
H176 = *"u^3 (A)"*
I176 = *"v^3 (B)"*
H177 = COMPLEX(I173,J174)
I177 = COMPLEX(I173,J175)
H178 = IMPOWER((H177,1/3)
I178 = IMPOWER(I177,1/3)
H179 = I173+J174
I179 = I173-J174
M180 = SIGN(H172)+1
N180 = SIGN(M180)
O180 = ABS(N180-1)
H181 = *"$\sqrt[3]{A}$"*
I181 = *"$\sqrt[3]{B}$"*
H182 = H179^(1/3)
I182 = I179^(1/3)
O182 = (2*O180)-1
M184 = A194*M172
F185 = *"If R is positive"*
G185 = *"If R is negative"*
M185 = M184+L172
A186 = *"w"*
B186 = *"w^2"*

E186 = *"1st Root"*
F186 = (H179^(1/3))+(I179^(1/3))-(C172/3)
G186 = B204
A187 = COMPLEX(-0.5,A189)
B187 = COMPLEX(-0.5,A190)
E187 = *"2nd Root"*
F187 = IMSUM((IMPRODUCT(A187,H182)),(IMPRODUCT(B187,I182)),(C172/-3))
G187 = C204
E188 = *"3rd Root"*
F188 = IMSUM((IMPRODUCT(B187,H182)),(IMPRODUCT(A187,I182)),(C172/-3))
G188 = D204
A189 = SQRT(3)/2
M189 = I172*M172
A190 = -A189
M190 = M189+L172
A193 = *"r"*
A194 = SQRT((-1/27)*(H172^3)*O182)
A195 = *"cos θ"*
B195 = *"θ"*
C195 = *"π"*
A196 = ((-0.5*M190)/M185)
B196 = (ACOS(A196))/((PI())*2)*360
C196 = PI()
F196 = *"Roots"*
F197 = IMSUM((IMPRODUCT(F186,L172)),(IMPRODUCT(G186,M172)))
B198 = *"θ / 3"*
F198 = IMSUM((IMPRODUCT(F187,L172)),(IMPRODUCT(G187,M172)))
B199 = B196/3
F199 = IMSUM((IMPRODUCT(F188,L172)),(IMPRODUCT(G188,M172)))
B201 = *"cos θ / 3"*
C201 = *"cos (θ + 360)/3"*
D201 = *"cos (θ + 720)/3"*
B202 = COS((B199/360)*(2*C196))
C202 = (2*(M185^(1/3))*COS((((B196+360)/3)/360)*2*C196))-(C172/3)
D202 = (2*(M185^(1/3))*COS((((B196+720)/3)/360)*2*C196))-(C172/3)
B204 = (2*(M185^(1/3))*B202)-(C172/3)
C204 = C202
D204 = D202

The following section solves the cubic equation for $[M] = 10^{-1}$ M

B208 = *"Normalized coefficient of x^3"*
C208 = *"Normalized coefficient of x^2"*
D208 = *"Normalized coefficient of x"*
E208 = *"Normalized constant"*
H208 = *"p"*
I208 = *"q"*
J208 = *"R"*
B209 = 1
C209 = C17/B17
D209 = D17/B17
E209 = -A7/B17
H209 = D209-((C209^2)/3)
I209 = E209-((C209*D209)/3)+((2/27)*C209^3))
J209 = ((1/27)*(H209^3))+(0.25*I209*I209)
K209 = SIGN(J209)+1
L209 = SIGN(K209)
M209 = ABS(L209-1)
I210 = -0.5*I209
J210 = SIGN(J209)*J209
J211 = SQRT(J210)

J212 = -1*J211
H213 = *"u^3 (A)"*
I213 = *"v^3 (B)"*
H214 = COMPLEX(I210,J211)
I214 = COMPLEX(I210,J212)
H215 = IMPOWER((H214,1/3)
I215 = IMPOWER(I214,1/3)
H216 = I210+J211
I216 = I210-J211
M217 = SIGN(H209)+1
N217 = SIGN(M217)
O217 = ABS(N217-1)
H218 = *"$\sqrt[3]{A}$"*
I218 = *"$\sqrt[3]{B}$"*
H219 = H216^(1/3)
I219 = I216^(1/3)
O219 = (2*O217)-1
M221 = A231*M209
F222 = *"If R is positive"*
G222 = *"If R is negative"*
M222 = M221+L209
A223 = *"w"*
B223 = *"w^2"*
E223 = *"1st Root"*
F223 = (H216^(1/3))+(I216^(1/3))-(C209/3)
G223 = B241
A224 = COMPLEX(-0.5,A226)
B224 = COMPLEX(-0.5,A227)
E224 = *"2nd Root"*
F224 = IMSUM((IMPRODUCT(A224,H219)),(IMPRODUCT(B224,I219)),(C209/-3))
G224 = C241
E225 = *"3rd Root"*
F225 = IMSUM((IMPRODUCT(B224,H219)),(IMPRODUCT(A224,I219)),(C209/-3))
G225 = D241
A226 = SQRT(3)/2
M226 = I209*M209
A227 = -A226
M227 = M226+L209
A230 = *"r"*
A231 = SQRT((-1/27)*(H209^3)*O219)
A232 = *"cos θ"*
B232 = *"θ"*
C232 = *"π"*
A233 = ((-0.5*M227)/M222)
B233 = (ACOS(A233))/((PI())*2)*360
C233 = PI()
F233 = *"Roots"*
F234 = IMSUM((IMPRODUCT(F223,L209)),(IMPRODUCT(G223,M209)))
B235 = *"θ / 3"*
F235 = IMSUM((IMPRODUCT(F224,L209)),(IMPRODUCT(G224,M209)))
B236 = B233/3
F236 = IMSUM((IMPRODUCT(F225,L209)),(IMPRODUCT(G225,M209)))
B238 = *"cos θ / 3"*
C238 = *"cos (θ + 360)/3"*
D238 = *"cos (θ + 720)/3"*
B239 = COS((B236/360)*(2*C233))
C239 = (2*(M222^(1/3))*COS((((B233+360)/3)/360)*2*C233))-(C209/3)
D239 = (2*(M222^(1/3))*COS((((B233+720)/3)/360)*2*C233))-(C209/3)
B241 = (2*(M222^(1/3))*B239)-(C209/3)
C241 = C239
D241 = D239

The following section solves the cubic equation for [*M*] = 1 M

B245 = *"Normalized coefficient of x^3"*
C245 = *"Normalized coefficient of x^2"*
D245 = *"Normalized coefficient of x"*
E245 = *"Normalized constant"*
H245 = *"p"*
I245 = *"q"*
J245 = *"R"*
B246 = 1
C246 = C17/B17
D246 = D17/B17
E246 = -A8/B17
H246 = D246-((C246^2)/3)
I246 = E246-((C246*D246)/3)+((2/27)*C246^3))
J246 = ((1/27)*(H246^3))+(0.25*I246*I246)
K246 = SIGN(J246)+1
L246 = SIGN(K246)
M246 = ABS(L246-1)
I247 = -0.5*I246
J247 = SIGN(J246)*J246
J248 = SQRT(J247)
J249 = -1*J248
H250 = *"u^3 (A)"*
I250 = *"v^3 (B)"*
H251 = COMPLEX(I247,J248)
I251 = COMPLEX(I247,J249)
H252 = IMPOWER((H251,1/3)
I252 = IMPOWER(I251,1/3)
H253 = I247+J248
I253 = I247-J248
M254 = SIGN(H246)+1
N254 = SIGN(M254)
O254 = ABS(N254-1)
H255 = *"$\sqrt[3]{A}$"*
I255 = *"$\sqrt[3]{B}$"*
H256 = H253^(1/3)
I256 = I253^(1/3)
O256 = (2*O254)-1
M258 = A268*M246
F259 = *"If R is positive"*
G259 = *"If R is negative"*
M259 = M258+L246
A260 = *"w"*
B260 = *"w^2"*
E260 = *"1st Root"*
F260 = (H253^(1/3))+(I253^(1/3))-(C246/3)
G260 = B278
A261 = COMPLEX(-0.5,A263)
B260 = COMPLEX(-0.5,A264)
E261 = *"2nd Root"*
F261 = IMSUM((IMPRODUCT(A261,H256)),(IMPRODUCT(B261,I256)),(C246/-3))
G261 = C278
E262 = *"3rd Root"*
F262 = IMSUM((IMPRODUCT(B261,H256)),(IMPRODUCT(A261,I256)),(C246/-3))
G262 = D278
A263 = SQRT(3)/2
M263 = I246*M246
A264 = -A263
M264 = M263+L246

A267 = *"r"*
A268 = SQRT((-1/27)*(H246^3)*O256)
A269 = *"cos θ"*
B269 = *"θ"*
C269 = *"π"*
A270 = ((-0.5*M264)/M259)
B270 = (ACOS(A270))/((PI())*2)*360
C270 = PI()
F270 = *"Roots"*
F271 = IMSUM((IMPRODUCT(F260,L246)),(IMPRODUCT(G260,M246)))
B272 = *"θ / 3"*
F272 = IMSUM((IMPRODUCT(F261,L246)),(IMPRODUCT(G261,M246)))
B273 = B270/3
F273 = IMSUM((IMPRODUCT(F262,L246)),(IMPRODUCT(G262,M246)))
B275 = *"cos θ / 3"*
C275 = *"cos (θ + 360)/3"*
D275 = *"cos (θ + 720)/3"*
B276 = COS((B273/360)*(2*C270))
C276 = (2*(M259^(1/3))*COS((((B270+360)/3)/360)*2*C270))-(C246/3)
D276 = (2*(M259^(1/3))*COS((((B270+720)/3)/360)*2*C270))-(C246/3)
B278 = (2*(M259^(1/3))*B276)-(C246/3)
C278 = C276
D278 = D276

The following section solves the cubic equation for [*M*] = 10 M

B283 = *"Normalized coefficient of x^3"*
C283 = *"Normalized coefficient of x^2"*
D283 = *"Normalized coefficient of x"*
E283 = *"Normalized constant"*
H283 = *"p"*
I283 = *"q"*
J283 = *"R"*
B284 = 1
C284 = C17/B17
D284 = D17/B17
E284 = -A9/B17
H284 = D284-((C284^2)/3)
I284 = E284-((C284*D284)/3)+((2/27)*C284^3))
J284 = ((1/27)*(H284^3))+(0.25*I284*I284)
K284 = SIGN(J284)+1
L284 = SIGN(K284)
M284 = ABS(L284-1)
I285 = -0.5*I284
J285 = SIGN(J284)*J284
J286 = SQRT(J285)
J287 = -1*J286
H288 = *"u^3 (A)"*
I288 = *"v^3 (B)"*
H289 = COMPLEX(I285,J286)
I289 = COMPLEX(I285,J287)
H290 = IMPOWER((H289,1/3)
I290 = IMPOWER(I289,1/3)
H291 = I285+J286
I291 = I285-J286
M292 = SIGN(H284)+1
N292 = SIGN(M292)
O292 = ABS(N292-1)
H293 = *"$\sqrt[3]{A}$"*
I293 = *"$\sqrt[3]{B}$"*
H294 = H291^(1/3)

I294 = I291^(1/3)
O294 = (2*O292)-1
M296 = A306*M284
F297 = *"If R is positive"*
G297 = *"If R is negative"*
M297 = M296+L284
A298 = *"w"*
B298 = *"w^2"*
E298 = *"1st Root"*
F298 = (H291^(1/3))+(I291^(1/3))-(C284/3)
G298 = B316
A299 = COMPLEX(-0.5,A301)
B299 = COMPLEX(-0.5,A302)
E299 = *"2nd Root"*
F299 = IMSUM((IMPRODUCT(A299,H294)),(IMPRODUCT(B299,I294)),(C284/-3))
G299 = C316
E300 = *"3rd Root"*
F300 = IMSUM((IMPRODUCT(B299,H294)),(IMPRODUCT(A299,I294)),(C284/-3))
G300 = D316
A301 = SQRT(3)/2
M301 = I284*M284
A302 = -A301
M302 = M301+L284
A305 = *"r"*
A306 = SQRT((-1/27)*(H284^3)*O294)
A307 = *"cos θ"*
B307 = *"θ"*
C307 = *"π"*
A308 = ((-0.5*M302)/M297)
B308 = (ACOS(A308))/((PI())*2)*360
C308 = PI()
F308 = *"Roots"*
F309 = IMSUM((IMPRODUCT(F298,L284)),(IMPRODUCT(G298,M284)))
B310 = *"θ / 3"*
F310 = IMSUM((IMPRODUCT(F299,L284)),(IMPRODUCT(G299,M284)))
B311 = B308/3
F311 = IMSUM((IMPRODUCT(F300,L284)),(IMPRODUCT(G300,M284)))
B313 = *"cos θ / 3"*
C313 = *"cos (θ + 360)/3"*
D313 = *"cos (θ + 720)/3"*
B314 = COS((B311/360)*(2*C308))
C314 = (2*(M297^(1/3))*COS((((B308+360)/3)/360)*2*C308))-(C284/3)
D314 = (2*(M297^(1/3))*COS((((B308+720)/3)/360)*2*C308))-(C284/3)
B316 = (2*(M297^(1/3))*B314)-(C284/3)
C316 = C314
D316 = D314

The following section solves the cubic equation for [*M*] = 100 M

B320 = *"Normalized coefficient of x^3"*
C320 = *"Normalized coefficient of x^2"*
D320 = *"Normalized coefficient of x"*
E320 = *"Normalized constant"*
H320 = *"p"*
I320 = *"q"*
J320 = *"R"*
B321 = 1
C321 = C17/B17
D321 = D17/B17
E321 = -A10/B17
H321 = D321-((C321^2)/3)

I321 = E321-((C321*D321)/3)+((2/27)*C321^3))
J321 = ((1/27)*(H321^3))+(0.25*I321*I321)
K321 = SIGN(J321)+1
L321 = SIGN(K321)
M321 = ABS(L321-1)
I322 = -0.5*I321
J322 = SIGN(J321)*J321
J323 = SQRT(J322)
J324 = -1*J323
H325 = "u^3 (A)"
I325 = "v^3 (B)"
H326 = COMPLEX(I322,J323)
I326 = COMPLEX(I322,J324)
H327 = IMPOWER((H326,1/3)
I327 = IMPOWER(I326,1/3)
H328 = I322+J323
I328 = I322-J323
M329 = SIGN(H321)+1
N329 = SIGN(M329)
O329 = ABS(N329-1)
H330 = "$\sqrt[3]{A}$"
I330 = "$\sqrt[3]{B}$"
H331 = H228^(1/3)
I331 = I328^(1/3)
O331 = (2*O329)-1
M336 = A343*M321
F334 = "If R is positive"
G334 = "If R is negative"
M334 = M333+L321
A335 = "w"
B335 = "w^2"
E335 = "1st Root"
F335 = (H328^(1/3))+(I328^(1/3))-(C321/3)
G335 = B353
A336 = COMPLEX(-0.5,A338)
B336 = COMPLEX(-0.5,A339)
E336 = "2nd Root"
F336 = IMSUM((IMPRODUCT(A336,H331)),(IMPRODUCT(B336,I331)),(C321/-3))
G336 = C353
E337 = "3rd Root"
F337 = IMSUM((IMPRODUCT(B336,H331)),(IMPRODUCT(A336,I331)),(C321/-3))
G337 = D353
A338 = SQRT(3)/2
M338 = I321*M321
A339 = -A338
M339 = M338+L321
A342 = "r"
A343 = SQRT((-1/27)*(H321^3)*O331)
A344 = "cos θ"
B344 = "θ"
C344 = "π"
A345 = ((-0.5*M339)/M334)
B345 = (ACOS(A345))/((PI())*2)*360
C345 = PI()
F345 = "Roots"
F346 = IMSUM((IMPRODUCT(F335,L321)),(IMPRODUCT(G335,M321)))
B347 = "θ / 3"
F347 = IMSUM((IMPRODUCT(F336,L321)),(IMPRODUCT(G336,M321)))
B348 = B345/3
F348 = IMSUM((IMPRODUCT(F337,L321)),(IMPRODUCT(G337,M321)))
B350 = "cos θ / 3"

C350 = *"cos (θ + 360)/3"*
D350 = *"cos (θ + 720)/3"*
B351 = COS((B348/360)*(2*C345))
C351 = (2*(M334^(1/3))*COS((((B345+360)/3)/360)*2*C345))-(C321/3)
D351 = (2*(M334^(1/3))*COS((((B345+720)/3)/360)*2*C345))-(C321/3)
B353 = (2*(M334^(1/3))*B351)-(C321/3)
C353 = C351
D353 = D351

The following section solves the cubic equation for the value of [*M*] entered into A11

B356 = *"Normalized coefficient of x^3"*
C356 = *"Normalized coefficient of x^2"*
D356 = *"Normalized coefficient of x"*
E356 = *"Normalized constant"*
H356 = *"p"*
I356 = *"q"*
J356 = *"R"*
B357 = 1
C357 = C17/B17
D357 = D17/B17
E357 = -A11/B17
H357 = D357-((C357^2)/3)
I357 = E357-((C357*D357)/3)+((2/27)*C357^3))
J357 = ((1/27)*(H357^3))+(0.25*I357*I357)
K357 = SIGN(J357)+1
L357 = SIGN(K357)
M357 = ABS(L357-1)
I358 = -0.5*I357
J358 = SIGN(J357)*J357
J359 = SQRT(J358)
J360 = -1*J359
H361 = *"u^3 (A)"*
I361 = *"v^3 (B)"*
H362 = COMPLEX(I358,J359)
I362 = COMPLEX(I358,J360)
H363 = IMPOWER((H362,1/3)
I363 = IMPOWER(I362,1/3)
H364 = I358+J359
I364 = I358-J359
M365 = SIGN(H357)+1
N365 = SIGN(M365)
O365 = ABS(N365-1)
H366 = *"$\sqrt[3]{A}$"*
I366 = *"$\sqrt[3]{B}$"*
H367 = H264^(1/3)
I367 = I364^(1/3)
O367 = (2*O365)-1
M369 = A379*M357
F370 = *"If R is positive"*
G370 = *"If R is negative"*
M370 = M369+L357
A371 = *"w"*
B371 = *"w^2"*
E371 = *"1st Root"*
F371 = (H364^(1/3))+(I364^(1/3))-(C357/3)
G371 = B389
A372 = COMPLEX(-0.5,A374)
B372 = COMPLEX(-0.5,A375)
E372 = *"2nd Root"*
F372 = IMSUM((IMPRODUCT(A372,H367)),(IMPRODUCT(B372,I367)),(C357/-3))

```
G372  =  C389
E373  =  "3rd Root"
F373  =  IMSUM((IMPRODUCT(B372,H367)),(IMPRODUCT(A372,I367)),(C357/-3))
G373  =  D389
A374  =  SQRT(3)/2
M374  =  I357*M357
A375  =  -A374
M375  =  M374+L357
A378  =  "r"
A379  =  SQRT((-1/27)*(H357^3)*O367)
A380  =  "cos θ"
B380  =  "θ"
C380  =  "π"
A381  =  ((-0.5*M375)/M370)
B381  =  (ACOS(A381))/((PI())*2)*360
C381  =  PI()
F381  =  "Roots"
F382  =  IMSUM((IMPRODUCT(F371,L357)),(IMPRODUCT(G371,M357)))
B383  =  "θ / 3"
F383  =  IMSUM((IMPRODUCT(F372,L357)),(IMPRODUCT(G372,M357)))
B384  =  B381/3
F384  =  IMSUM((IMPRODUCT(F373,L357)),(IMPRODUCT(G373,M357)))
B386  =  "cos θ / 3"
C386  =  "cos (θ + 360)/3"
D386  =  "cos (θ + 720)/3"
B387  =  COS((B384/360)*(2*C381))
C387  =  (2*(M370^(1/3))*COS((((B381+360)/3)/360)*2*C381))-(C357/3)
D387  =  (2*(M370^(1/3))*COS((((B381+720)/3)/360)*2*C381))-(C357/3)
B389  =  (2*(M370^(1/3))*B387)-(C357/3)
C389  =  C387
D389  =  D387
```

The output from this spreadsheet is a plot of how the concentration of each monomer/oligomer present in solution varies with the concentration of dissolved monomer. The *x* axis is a log scale of the dissolved monomer concentration [*M*], and the *y* axis is the percentage of any one particular species expressed as its molar concentration divided by the total concentration of all species present in solution. It should be noted that the sum total of the concentrations of all species present in solution will be less than the value of [*M*], unless there is no oligomerization whatsoever, in which case the value will, obviously, be [*M*]. For example, if 100 mM of monomer is dissolved in solution, and forms exclusively the [*c*2]daisy chain, the total concentration of all species present in solution is 50 mM. The *x* values are taken from cells B2–10, and the six sets of *y* axis data originate from cells L2–10, M2–10, N2–10, O2–10, P2–10, Q2–10, respectively.