Tab_Per_1 – how to plot 3-D atomic radii on the periodic table

```
clear all;clc;format short;format compact;
d = 0.18; % clearance

figure(1,'position',[100 100 1000 800]);
axis([0 18 0 18 0 300]);axis on;grid on;grid minor on;xticks(20);yticks(20);

AtNo = [0 18;17 18;0 17;1 17;12 17;13 17;14 17;15 17;16 17;17 17;... % x(i),y(i)
        0 16;1 16;12 16;13 16;14 16;15 16;16 16;17 16;...
        0 15;1 15;2 15;3 15;4 15;5 15;6 15;7 15;8 15;9 15;10 15;11 15;12 15;13 15;14 15;15 15;16 15;17 15;...
        0 14;1 14;2 14;3 14;4 14;5 14;6 14;7 14;8 14;9 14;10 14;11 14;12 14;13 14;14 14;15 14;16 14;17 14;...
        0 13;1 13;2 10;3 10;4 10;5 10;6 10;7 10;8 10;9 10;10 10;11 10;12 10;13 10;14 10;15 10;...
        2 13;3 13;4 13;5 13;6 13;7 13;8 13;9 13;10 13;11 13;12 13;13 13;14 13;15 13;16 13;17 13;...
        0 12;1 12;2 9;3 9;4 9;5 9;6 9;7 9;8 9;9 9;10 9;11 9;12 9;13 9;14 9;15 9;...
        2 12;3 12;4 12;5 12;6 12;7 12;8 12;9 12;10 12;11 12;12 12;13 12;14 12;15 12;16 12;17 12];
% The following line is to be used once. When the file id downloaded, inactivate the line by adding % (remark symbol)
f = urlwrite('www.molecularmodels.eu/atomicRadius.txt','atomicRadius.txt');

A = importdata("atomicRadius.txt","\n");
ln = length(A)
for i=1:ln
  b = strsplit(A{i});
  nAt = str2num(b{1});eNeg = str2num(b{4});h1 = eNeg;
  x1 = AtNo(nAt,1) + d;y1 = AtNo(nAt,2) - d;x2 = x1 + 1 - d;y2 = y1 -1 + d;
  v2 = [x1 y1 0;x2 y1 0;x2 y2 0;x1 y2 0;x1 y1 h1;x2 y1 h1;x2 y2 h1;x1 y2 h1];
  f2 = [3 4 8 7;1 4 8 5;5 6 7 8];
  patch('Faces',f2,'Vertices',v2,'FaceColor',[(h1/300) 0 (1-h1/300)]);view(3);
endfor

xlabel("groups",'FontSize',20);ylabel("periods",'FontSize',20);zlabel("Atomic Radius (pm)",'FontSize',20);
title("Atomic Radius (calculated)",'FontSize',20);

for i=0.5:17.5
  text(i-0.2,7,0.6,num2str(i+0.5),'FontSize',20);
endfor
for i=18:-1:12
  text(-1.3,i-1,num2str(19-i),'FontSize',20);
endfor
```

SeaWaterCalc – a complete script for seawater equilibria

```
clear;clc;
global SO4 KS K1 K2 Kw K7 K8 H2CO3 HCO3 CO3 OH F KF KB B BOH4 Ksp1 pptF Mg Sr Na K Cl Br H HT
global Hsws Ca
% No Mg(OH)+ or Ca(OH)+ formation because they seem to have neglegible effects
function y = neut(pH) % ===> pH free scale, i.e. chemical true scale, always used if not otherwise stated !!
    global SO4 KS K1 K2 Kw K7 K8 H2CO3 HCO3 CO3 OH F KF KB B BOH4 Ksp1 pptF Mg Sr Na K Cl Br H HT
    global Hsws Ca
    H = 10^(-pH);
    HCO3 = K1*H2CO3/H;
    CO3 = K2*HCO3/H;
    HF = H*F/(KF + H);
    HSO4 = H*SO4/(KS + H);
    Hsws = H + HF + HSO4;  % ===> pH SWS scale only here
    OH = Kw/Hsws;          % ===> pH SWS scale only here
    HT = H + HSO4;         % ===> pH total scale only here
    BOH4 = KB*B/(HT + KB); % ===> pH total scale only here
    y = H - OH  + 2*Ca + 2*Mg + 2*Sr + Na + K - 2*(SO4-HSO4) - BOH4 - HCO3 - 2*CO3 - Cl - (F-HF) - Br - HSO4;
endfunction

Cini = 0;
% Display of data in condensed form is prepared.
disp('Temp = temperature in degree Celsius (°C)');
disp('CO2  = ppmv, parts per million in volume of CO2 in dry air');
disp('pptF = fraction of CaCO3(calcite) which precipitates, ratio to complete precipitation(when omega=1)');
disp('Pres = pressure in atm x 100');
disp('Saln = salinity in grams of dissoved salts per kg of solution');
disp('pHfr. pHtot pHsws = different pH scales, free, total and seawater');
disp('pOH  = -log10[OH-]');
disp('H2CO3  HCO3  CO3 = concentrations in millimol/kg-solution');
disp('DIC  = Dissolved Inorganic Carbon in mmol/kg-soln');
disp('Alk  = alkalinity in mmol/kg-soln  Alk = 2*CO3+HCO3+OH+BOH4-H');
disp('Ca++ CaCO3   = concentrations in mmol/kg-soln');
disp('sovr1  sovr2 = Calcite and aragonite overasaturation (omega)');
disp('pH2O = water vapour pressure above sea level');
disp('Cout = mmol/kg-soln of carbon absorbed(-) or outgassed (+) from the first iteration');
T0 =['|Temp|CO2|pptF|Pres|Saln|pHfr.|pHtot|pHsws| pOH |H2CO3 |HCO3-|CO3-- | DIC | Ca++ | Alk |CaCO3|over1|over2| pH2O | Cout'];
T2 =['+----+---+----+----+----+-----+-----+-----+-----+------+-----+------+-----+------+-----+-----+-----+------+'];
disp(T2);disp(T0);disp(T2);
%*************************************************************************
% --> HERE AS FOLLOWS THE 6 PARAMETERS. THEY CAN BE VARIED IN A REASONABLE RANGE*
Tc = 17;         % temperature in Celsius (°C)                              *
ppmCO2 = 285;    % parts per million (in volume) of CO2 in the atmosphere   *
```

```
P = 0;           % pressure in atm. P=0 means ambient pressure, 1 atm.          *
S = 35;          % salinity, in grams of salts in 1 kg of solution              *
pptF = 0;        % fraction of CaCO3 which actually precipitates                *
pH2O =  100;     % H2O vapour pressure in %saturation at sea level              *
%*****************************************************************************
%  standard seawater composition for salinity = 35 g/Kg-soln
 Cli  = 0.54586;     % Cl-   Mol/kg(solution)
 Nai  = 0.46906;     % Na+   Mol/kg(solution)
 Mgi  = 0.05282;     % Mg++  Mol/kg(solution)
 Cai  = 0.01028;     % Ca++  Mol/kg(solution)
 SO4i = 0.02824;     % SO4-- Mol/kg(solution)
 Ki   = 0.01021;     % K+    Mol/kg(solution)
 Bri  = 0.00084;     % Br-   Mol/kg(solution)
 Sri  = 0.00009;     % Sr++  Mol/kg(solution)
 Fi   = 0.00007;     % F-    Mol/kg(solution)
 Bi   = 0.00042;     % B(OH)3 + B(OH)4- Mol/kg(solution)

%  standard seawater composition is corrected for salinity
 Cl = Cli*S/35;Na = Nai*S/35;Mg = Mgi*S/35;Ca = Cai*S/35;SO4 = SO4i*S/35;
 K = Ki*S/35;Br = Bri*S/35;Sr = Sri*S/35;F = Fi*S/35;B = Bi*S/35;

 R = 8.314;R1 = 83.131;j = 0;CaCO3Tot = 0;
%*****************************************************************************

% -----> For/Endfor cycle for one of the five parameters Tc, ppmCO2, P, pptF, pH2O
for ppmCO2 = 280:10:580 % modify line to cycle over other parameters

T = Tc + 273.15;

% CO2 + H2O <==> H2CO3 (Weiss 1994)
LnK0 = 9345.17/T - 60.2409 + 23.3585*log(T/100) + S*(0.023517 - 0.00023656*T + 0.0047036*(T/100)^2);

% H2CO3 <==> H+ + HCO3-
% --> Waters, Millero, Woosley (Mar. Chem., 165, 66-67, 2014)  [H+]=free scale
LnK1 = -log(10)*(6320.813/T + 19.568224*log(T) -126.34048 + 5.592953*S^0.5 + 0.028845*S - (6.388e-5)*S^2 + (-225.7489*S^0.5 -
4.761*S)/T -0.8715109*S^0.5*log(T));
% HCO3- <==> H+ + CO3--
% --> Waters, Millero, Woosley (Mar. Chem., 165, 66-67, 2014)  [H+]=free scale
LnK2 = -log(10)*(5143.692/T + 14.613358*log(T) - 90.18333 + 13.396949*S^0.5 + 0.12193009*S - (3.8362e-4)*S^2 + (-472.8633*S^0.5 -
19.03634*S)/T - 2.1563270*S^0.5*log(T));

% H2O <==> H+ + OH- (DOE 1994)  % pH = pH(SWS) !!
LnKw = 148.9802 - 13847.26/T - 23.6521*log(T) + (118.67/T - 5.977 + 1.0495*log(T))*S^0.5 - 0.01615*S;
```

```
% HSO4- <==> H+ + SO4--
I = 19.924*S/(1000 - 1.005*S); % ionic strenght, useful for KS and KF calculations
LnKS = -4276.1/T + 141.328 - 23.039*log(T) + (-13856/T + 324.57  - 47.986*log(T))*I^0.5 + (35474/T - 771.54 + 114.723*log(T))*I -
2698/T*I^1.5 + 1766/T*I^2 + log(1-0.001005*S);

% HF <==> H+ + F-
LnKF = 1590.2/T - 12.641 + 1.525*I^0.5 + log(1-0.001005*S);  % pH = pH free NO conversion to total

% CaCO3calcite <==> Ca++ + CO3--
LogKspCal = -171.9065 - 0.077993*T + 2839.319/T + 71.595*log10(T) + (-0.77712 + 0.0028426*T + 178.34/T)*S^0.5 - 0.07711*S +
0.0041249*S^1.5;
LnKspCal = LogKspCal*log(10);

% CaCO3aragonite <==> Ca++ + CO3--
LogKspAra = -171.945 - 0.077993*T + 2903.293/T + 71.595*log10(T) + (-0.068393 + 0.0017276*T + 88.135/T)*S^0.5 - 0.10018*S +
0.0059415*S^1.5;
LnKspAra = LogKspAra*log(10);

% B(OH)3 + H2O <==> H+ + B(OH)4-
LnKB = (-8966.9 - 2890.53*S^0.5 - 77.942*S + 1.728*S^1.5 - 0.0996*S^2)/T + 148.0248 + 137.1942*S^0.5 + 1.62142*S - (24.4344 +
25.085*S^0.5 + 0.2474*S)*log(T) + 0.053105*S^0.5*T;

% The log(K) are modified according to hydrostatic pressure (on the sea surface P=0)
LnK1P = LnK1 + (25.5 - 0.1271*Tc)/R1/T*P + 0.5*(-3.08e-3 + 0.0877e-3*Tc)/R1/T*P^2;
LnK2P = LnK2 + (15.82 + 0.0219*Tc)/R1/T*P + 0.5*(1.13e-3 - 0.1475e-3*Tc)/R1/T*P^2;
LnKwP = LnKw + (25.6 - 0.2324*Tc + 3.6246e-3*Tc^2)/R1/T*P + 0.5*(-5.13e-3 + 0.0794e-3*Tc)/R1/T*P^2;
LnKBP = LnKB + (29.48 - 0.1622*Tc - 2.608e-3*Tc^2)/R1/T*P + 0.5*(-2.84e-3)/R1/T*P^2;
LnKspCalP = LnKspCal + (48.76 - 0.5304*Tc)/R1/T*P + 0.5*(-11.76e-3 + 0.3692e-3*Tc )/R1/T*P^2;
LnKspAraP = LnKspAra + (46 - 0.5304*Tc)/R1/T*P + 0.5*(-11.76e-3 + 0.3692e-3*Tc)/R1/T*P^2;
LnKSP = LnKS + (18.03 - 0.0466*Tc - 0.3160e-3*Tc^2)/R1/T*P + 0.5*(-4.53e-3 + 0.09e-3*Tc)/R1/T*P^2;
LnKFP = LnKF + (9.78 + 0.009*Tc + 0.942e-3*Tc^2)/R1/T*P + 0.5*(-3.91e-3 + 0.054*Tc)/R1/T*P^2;
% The K(eq) values are calculated from their logarithms.
K1 = exp(LnK1P);K2 = exp(LnK2P);K0 = exp(LnK0);Kw = exp(LnKwP);Ksp1 = exp(LnKspCalP);
Ksp2 = exp(LnKspAraP);KS = exp(LnKSP);KF = exp(LnKFP);KB = exp(LnKBP);
% CO2 fugacity is introduced, according to Koertzinger (pag 65 Zeebe and Gladrow 2001)
fCO2 = ppmCO2*exp(101325*((-1636.75 + 12.0408*T - 3.27957e-2*T^2 + 3.16528e-5*T^3)*1e-6 + 2*(57.7 - 0.118*T)*1e-6)/R/T);
% H2O vapour pressure is calculated for seawater, Weiss and Price 1980
LnpH2O = 24.4543 -6745.09/T - 4.8489*log(T/100) -0.000544*S;
% CO2 fugacity is corrected according to water vapour partial pressure
fCO2 = fCO2*(1 - exp(LnpH2O)*pH2O/100);
H2CO3 = K0*fCO2*1e-6;

[pH,fval,info] = fzero(@neut,[0,14]); % call to fzero
s = roots([1,-(Ca + CO3),Ca*CO3 - Ksp1]); % CaCO3 calcite solubility check
```

```
% according to solubility product [Ca++]·[CO3--] = Ksp1
% equilibrium is reached when [Ca-x]·[CO3-x] = Ksp1   ; where x = CaCO3 amount formed in 1 kg of solution.
% funcion 'roots' solves the second order equation above. CaCO3 formed is modulated by pptF, usually 0 <= pptF <= 0.1
% pptF = 0 means no calcite (CaCO3) is formed.
CaCO3 = s(2)*pptF*1000;              %  Calcite is formed according to pptF
CaCO3Tot = CaCO3Tot + CaCO3;         %  Formed calcite is added to bulk
DIC = (H2CO3+HCO3+CO3)*1000;         %  Dissolved Inorganic Carbon in mmol/kg-soln
Alk = 1000*(2*CO3+HCO3+OH+BOH4-H);   %  Total Alkalinity mmol/kg-soln
OverSatCal = Ca*CO3/Ksp1;            %  Oversaturation of CaCO3 (calcite form)
OverSatAra = Ca*CO3/Ksp2;            %  Oversaturation of CaCO3 (aragonite form)
if Cini == 0;Cini = 1000*(H2CO3 + HCO3 + CO3) + CaCO3Tot;end  %DIC iniziale
Cout = Cini - 1000*(H2CO3 + HCO3 + CO3) - CaCO3Tot;           %CO2 outgassed during the for/endfor cycles

% In the iterative procedure, CaCO3 is detracted from Ca++ in solution each step ?
% Ca = Ca - CaCO3/1000; % if this line is active, yes ;but it is not realistic and it's better to leave the line commented (%)

% The results are displayed.
if Tc<10;T1 = ['|',num2str(Tc,'%.2f')];else T1 =['|',num2str(Tc,'%.1f')];endif
T1 = [T1,'|',num2str(ppmCO2,3),'|',num2str(pptF,'%.2f'),'|',num2str(P/100,'%.2f'),'|',num2str(S,'%.1f')];
T1 = [T1,'|',num2str(pH,'%.3f'),'|',num2str(-log10(HT),'%.3f'),'|',num2str(-log10(Hsws),'%.3f'),'|',num2str(-log10(OH),'%.3f')];
T1 = [T1,'|',num2str(H2CO3*1000,'%.4f'),'|',num2str(HCO3*1000,'%.3f'),'|',num2str(CO3*1000,'%.4f')];
T1 = [T1,'|',num2str(DIC,'%.3f'),'|'];
if Ca>0.01;T1 = [T1, num2str(Ca*1000,'%.3f')];else;T1 = [T1, num2str(Ca*1000,'%.4f')];endif
T1 = [T1,'|',num2str(Alk,'%.3f'),'|',num2str(CaCO3Tot,'%.3f'),'|',num2str(OverSatCal,'%.3f')];
T1 = [T1,'|',num2str(OverSatAra,'%.3f'),'|',num2str(exp(LnpH2O),'%.4f'),'|',num2str(Cout,'%.2f')];
disp(T1);
++j;
x(j) = DIC;y1(j) = ppmCO2;  % modify line to plot other variables
endfor
disp(T2);
plot(x,y1,'r','LineWidth',2);grid on;grid minor on;xlabel('DIC(mmol/kg)');ylabel('ppmCO2');hold on;
title('ppmCO2 versus Dissolved Inorganic Carbon @17°C (avg. seawater temp.)')
```

Some text output examples are listed in the following:

1) Temperature ranging from 0 to 30 °C while all other 5 parameters remain as default

Temp	CO2	pptF	Pres	Saln	pHfr.	pHtot	pHsws	pOH	H2CO3	HCO3-	CO3--	DIC	Ca++	Alk	CaCO3	over1	over2	pH2O	Cout
0.00	410	0.00	0.00	35.0	8.099	8.068	8.061	6.239	0.0255	2.149	0.0989	2.274	10.280	2.400	0.000	2.369	1.489	0.0059	0.00
1.00	410	0.00	0.00	35.0	8.102	8.070	8.062	6.189	0.0245	2.139	0.1028	2.267	10.280	2.400	0.000	2.461	1.548	0.0064	0.01
2.00	410	0.00	0.00	35.0	8.106	8.072	8.064	6.139	0.0236	2.130	0.1069	2.260	10.280	2.400	0.000	2.556	1.609	0.0068	0.01

|3.00|410|0.00|0.00|35.0|8.109|8.073|8.066|6.090|0.0227|2.119|0.1111|2.253|10.280|2.400|0.000|2.653|1.672|0.0073|0.02
|4.00|410|0.00|0.00|35.0|8.112|8.075|8.067|6.041|0.0219|2.109|0.1153|2.246|10.280|2.400|0.000|2.753|1.736|0.0079|0.03
|5.00|410|0.00|0.00|35.0|8.115|8.076|8.068|5.993|0.0211|2.098|0.1197|2.239|10.280|2.400|0.000|2.855|1.803|0.0084|0.03
|6.00|410|0.00|0.00|35.0|8.118|8.078|8.070|5.946|0.0204|2.088|0.1241|2.232|10.280|2.400|0.000|2.959|1.871|0.0090|0.04
|7.00|410|0.00|0.00|35.0|8.121|8.079|8.071|5.898|0.0196|2.077|0.1287|2.225|10.280|2.400|0.000|3.066|1.941|0.0097|0.05
|8.00|410|0.00|0.00|35.0|8.125|8.080|8.072|5.852|0.0190|2.065|0.1333|2.218|10.280|2.400|0.000|3.176|2.013|0.0104|0.06
|9.00|410|0.00|0.00|35.0|8.128|8.081|8.073|5.806|0.0183|2.054|0.1381|2.210|10.280|2.400|0.000|3.288|2.088|0.0111|0.06
|10.0|410|0.00|0.00|35.0|8.131|8.082|8.074|5.760|0.0177|2.042|0.1429|2.203|10.280|2.400|0.000|3.402|2.164|0.0119|0.07
|11.0|410|0.00|0.00|35.0|8.133|8.083|8.075|5.715|0.0171|2.030|0.1478|2.195|10.280|2.400|0.000|3.519|2.242|0.0127|0.08
|12.0|410|0.00|0.00|35.0|8.136|8.084|8.075|5.671|0.0166|2.018|0.1528|2.188|10.280|2.400|0.000|3.639|2.323|0.0136|0.09
|13.0|410|0.00|0.00|35.0|8.139|8.085|8.076|5.626|0.0160|2.006|0.1580|2.180|10.280|2.400|0.000|3.761|2.405|0.0145|0.09
|14.0|410|0.00|0.00|35.0|8.142|8.086|8.077|5.583|0.0155|1.993|0.1632|2.172|10.280|2.400|0.000|3.886|2.490|0.0155|0.10
|15.0|410|0.00|0.00|35.0|8.145|8.086|8.077|5.540|0.0151|1.981|0.1684|2.164|10.280|2.400|0.000|4.013|2.577|0.0165|0.11
|16.0|410|0.00|0.00|35.0|8.148|8.087|8.077|5.497|0.0146|1.968|0.1738|2.156|10.280|2.400|0.000|4.143|2.666|0.0176|0.12
|17.0|410|0.00|0.00|35.0|8.150|8.087|8.078|5.455|0.0141|1.954|0.1793|2.148|10.280|2.400|0.000|4.275|2.758|0.0187|0.13
|18.0|410|0.00|0.00|35.0|8.153|8.088|8.078|5.413|0.0137|1.941|0.1848|2.140|10.280|2.400|0.000|4.410|2.852|0.0200|0.13
|19.0|410|0.00|0.00|35.0|8.156|8.088|8.078|5.372|0.0133|1.928|0.1904|2.131|10.280|2.400|0.000|4.548|2.948|0.0213|0.14
|20.0|410|0.00|0.00|35.0|8.158|8.088|8.078|5.331|0.0129|1.914|0.1961|2.123|10.280|2.400|0.000|4.688|3.047|0.0226|0.15
|21.0|410|0.00|0.00|35.0|8.161|8.088|8.078|5.291|0.0126|1.900|0.2018|2.114|10.280|2.400|0.000|4.830|3.148|0.0241|0.16
|22.0|410|0.00|0.00|35.0|8.163|8.088|8.078|5.251|0.0122|1.886|0.2077|2.106|10.280|2.400|0.000|4.975|3.251|0.0256|0.17
|23.0|410|0.00|0.00|35.0|8.166|8.088|8.078|5.211|0.0119|1.872|0.2135|2.097|10.280|2.400|0.000|5.123|3.357|0.0272|0.18
|24.0|410|0.00|0.00|35.0|8.168|8.088|8.078|5.172|0.0116|1.857|0.2195|2.088|10.280|2.400|0.000|5.273|3.465|0.0289|0.19
|25.0|410|0.00|0.00|35.0|8.171|8.088|8.077|5.134|0.0112|1.842|0.2255|2.079|10.280|2.400|0.000|5.426|3.577|0.0307|0.19
|26.0|410|0.00|0.00|35.0|8.173|8.087|8.077|5.095|0.0109|1.828|0.2316|2.070|10.280|2.400|0.000|5.582|3.690|0.0325|0.20
|27.0|410|0.00|0.00|35.0|8.176|8.087|8.076|5.057|0.0107|1.813|0.2377|2.061|10.280|2.400|0.000|5.739|3.807|0.0345|0.21
|28.0|410|0.00|0.00|35.0|8.178|8.087|8.076|5.020|0.0104|1.798|0.2439|2.052|10.280|2.400|0.000|5.900|3.926|0.0366|0.22
|29.0|410|0.00|0.00|35.0|8.180|8.086|8.075|4.983|0.0101|1.782|0.2501|2.042|10.280|2.400|0.000|6.063|4.047|0.0388|0.23
|30.0|410|0.00|0.00|35.0|8.183|8.086|8.074|4.946|0.0099|1.767|0.2564|2.033|10.280|2.400|0.000|6.228|4.172|0.0411|0.24

2) ppmCO2 ranging from 300 to 500 (step : 10) while all other 5 parameters remain as default

|Temp|CO2|pptF|Pres|Saln|pHfr.|pHtot|pHsws| pOH |H2CO3 |HCO3-|CO3-- | DIC | Ca++ | Alk |CaCO3|over1|over2| pH2O | Cout
|4.00|300|0.00|0.00|35.0|8.231|8.194|8.186|5.922|0.0160|2.032|0.1462|2.194|10.280|2.400|0.000|3.491|2.201|0.0079|0.00
|4.00|310|0.00|0.00|35.0|8.219|8.182|8.174|5.934|0.0166|2.040|0.1427|2.200|10.280|2.400|0.000|3.407|2.149|0.0079|-0.01
|4.00|320|0.00|0.00|35.0|8.207|8.170|8.162|5.946|0.0171|2.049|0.1394|2.205|10.280|2.400|0.000|3.328|2.099|0.0079|-0.01
|4.00|330|0.00|0.00|35.0|8.195|8.158|8.150|5.958|0.0176|2.057|0.1362|2.210|10.280|2.400|0.000|3.252|2.051|0.0079|-0.02
|4.00|340|0.00|0.00|35.0|8.184|8.147|8.139|5.969|0.0182|2.064|0.1332|2.216|10.280|2.400|0.000|3.180|2.005|0.0079|-0.02
|4.00|350|0.00|0.00|35.0|8.173|8.136|8.128|5.980|0.0187|2.071|0.1303|2.220|10.280|2.400|0.000|3.111|1.962|0.0079|-0.03
|4.00|360|0.00|0.00|35.0|8.162|8.125|8.117|5.991|0.0192|2.078|0.1275|2.225|10.280|2.400|0.000|3.044|1.920|0.0079|-0.03
|4.00|370|0.00|0.00|35.0|8.152|8.114|8.107|6.002|0.0198|2.085|0.1249|2.230|10.280|2.400|0.000|2.981|1.880|0.0079|-0.04
|4.00|380|0.00|0.00|35.0|8.141|8.104|8.096|6.012|0.0203|2.091|0.1223|2.234|10.280|2.400|0.000|2.921|1.842|0.0079|-0.04

|4.00|390|0.00|0.00|35.0|8.131|8.094|8.086|6.022|0.0208|2.098|0.1199|2.238|10.280|2.400|0.000|2.862|1.805|0.0079|-0.04
|4.00|400|0.00|0.00|35.0|8.122|8.084|8.077|6.032|0.0214|2.103|0.1176|2.242|10.280|2.400|0.000|2.806|1.770|0.0079|-0.05
|4.00|410|0.00|0.00|35.0|8.112|8.075|8.067|6.041|0.0219|2.109|0.1153|2.246|10.280|2.400|0.000|2.753|1.736|0.0079|-0.05
|4.00|420|0.00|0.00|35.0|8.103|8.065|8.058|6.051|0.0224|2.114|0.1131|2.250|10.280|2.400|0.000|2.701|1.704|0.0079|-0.06
|4.00|430|0.00|0.00|35.0|8.094|8.056|8.049|6.060|0.0230|2.120|0.1111|2.254|10.280|2.400|0.000|2.651|1.672|0.0079|-0.06
|4.00|440|0.00|0.00|35.0|8.085|8.047|8.040|6.069|0.0235|2.125|0.1091|2.257|10.280|2.400|0.000|2.603|1.642|0.0079|-0.06
|4.00|450|0.00|0.00|35.0|8.076|8.039|8.031|6.077|0.0240|2.130|0.1071|2.261|10.280|2.400|0.000|2.557|1.613|0.0079|-0.07
|4.00|460|0.00|0.00|35.0|8.067|8.030|8.022|6.086|0.0246|2.134|0.1053|2.264|10.280|2.400|0.000|2.513|1.585|0.0079|-0.07
|4.00|470|0.00|0.00|35.0|8.059|8.022|8.014|6.094|0.0251|2.139|0.1035|2.267|10.280|2.400|0.000|2.470|1.558|0.0079|-0.07
|4.00|480|0.00|0.00|35.0|8.051|8.013|8.006|6.103|0.0256|2.143|0.1017|2.271|10.280|2.400|0.000|2.428|1.531|0.0079|-0.08
|4.00|490|0.00|0.00|35.0|8.043|8.005|7.997|6.111|0.0262|2.147|0.1000|2.274|10.280|2.400|0.000|2.388|1.506|0.0079|-0.08
|4.00|500|0.00|0.00|35.0|8.035|7.997|7.989|6.119|0.0267|2.152|0.0984|2.277|10.280|2.400|0.000|2.349|1.482|0.0079|-0.08

3) Pressure ranging from 0 to 600 bar(step : 20) while all other 5 parameters remain as default

|Temp|CO2|pptF|Pres|Saln|pHfr.|pHtot|pHsws| pOH |H2CO3 |HCO3-|CO3-- | DIC | Ca++ | Alk |CaCO3|over1|over2| pH2O | Cout
|4.00|410|0.00|0.00|35.0|8.112|8.075|8.067|6.041|0.0219|2.109|0.1153|2.246|10.280|2.400|0.000|2.753|1.736|0.0079|0.00
|4.00|410|0.00|0.20|35.0|8.103|8.066|8.058|6.041|0.0219|2.110|0.1145|2.247|10.280|2.400|0.000|2.626|1.660|0.0079|-0.00
|4.00|410|0.00|0.40|35.0|8.094|8.058|8.050|6.040|0.0219|2.112|0.1138|2.247|10.280|2.400|0.000|2.506|1.588|0.0079|-0.00
|4.00|410|0.00|0.60|35.0|8.085|8.049|8.042|6.039|0.0219|2.113|0.1130|2.248|10.280|2.400|0.000|2.392|1.519|0.0079|-0.00
|4.00|410|0.00|0.80|35.0|8.076|8.040|8.033|6.038|0.0219|2.114|0.1123|2.248|10.280|2.400|0.000|2.283|1.454|0.0079|-0.00
|4.00|410|0.00|1.00|35.0|8.066|8.032|8.025|6.037|0.0219|2.115|0.1116|2.249|10.280|2.400|0.000|2.180|1.392|0.0079|-0.00
|4.00|410|0.00|1.20|35.0|8.057|8.023|8.016|6.037|0.0219|2.116|0.1109|2.249|10.280|2.400|0.000|2.082|1.332|0.0079|-0.00
|4.00|410|0.00|1.40|35.0|8.048|8.015|8.008|6.036|0.0219|2.118|0.1101|2.250|10.280|2.400|0.000|1.989|1.276|0.0079|-0.00
|4.00|410|0.00|1.60|35.0|8.039|8.006|8.000|6.035|0.0219|2.119|0.1094|2.250|10.280|2.400|0.000|1.901|1.222|0.0079|-0.00
|4.00|410|0.00|1.80|35.0|8.030|7.998|7.991|6.035|0.0219|2.120|0.1088|2.250|10.280|2.400|0.000|1.817|1.171|0.0079|-0.00
|4.00|410|0.00|2.00|35.0|8.021|7.989|7.983|6.034|0.0219|2.121|0.1081|2.251|10.280|2.400|0.000|1.736|1.122|0.0079|-0.00
|4.00|410|0.00|2.20|35.0|8.012|7.981|7.975|6.033|0.0219|2.122|0.1074|2.251|10.280|2.400|0.000|1.660|1.075|0.0079|-0.01
|4.00|410|0.00|2.40|35.0|8.003|7.972|7.967|6.032|0.0219|2.123|0.1067|2.252|10.280|2.400|0.000|1.588|1.031|0.0079|-0.01
|4.00|410|0.00|2.60|35.0|7.994|7.964|7.958|6.032|0.0219|2.124|0.1061|2.252|10.280|2.400|0.000|1.519|0.988|0.0079|-0.01
|4.00|410|0.00|2.80|35.0|7.986|7.955|7.950|6.031|0.0219|2.125|0.1054|2.253|10.280|2.400|0.000|1.453|0.948|0.0079|-0.01
|4.00|410|0.00|3.00|35.0|7.977|7.947|7.942|6.031|0.0219|2.126|0.1048|2.253|10.280|2.400|0.000|1.391|0.909|0.0079|-0.01
|4.00|410|0.00|3.20|35.0|7.968|7.938|7.934|6.030|0.0219|2.127|0.1042|2.253|10.280|2.400|0.000|1.331|0.872|0.0079|-0.01
|4.00|410|0.00|3.40|35.0|7.959|7.930|7.926|6.030|0.0219|2.128|0.1035|2.254|10.280|2.400|0.000|1.274|0.837|0.0079|-0.01
|4.00|410|0.00|3.60|35.0|7.950|7.921|7.917|6.029|0.0219|2.129|0.1029|2.254|10.280|2.400|0.000|1.220|0.804|0.0079|-0.01
|4.00|410|0.00|3.80|35.0|7.941|7.913|7.909|6.029|0.0219|2.130|0.1023|2.254|10.280|2.400|0.000|1.169|0.771|0.0079|-0.01
|4.00|410|0.00|4.00|35.0|7.932|7.904|7.901|6.028|0.0219|2.131|0.1017|2.255|10.280|2.400|0.000|1.120|0.741|0.0079|-0.01
|4.00|410|0.00|4.20|35.0|7.923|7.896|7.893|6.028|0.0219|2.132|0.1011|2.255|10.280|2.400|0.000|1.073|0.712|0.0079|-0.01
|4.00|410|0.00|4.40|35.0|7.915|7.887|7.885|6.027|0.0219|2.133|0.1005|2.255|10.280|2.400|0.000|1.028|0.684|0.0079|-0.01
|4.00|410|0.00|4.60|35.0|7.906|7.879|7.876|6.027|0.0219|2.134|0.0999|2.256|10.280|2.400|0.000|0.986|0.657|0.0079|-0.01
|4.00|410|0.00|4.80|35.0|7.897|7.871|7.868|6.027|0.0219|2.135|0.0994|2.256|10.280|2.400|0.000|0.945|0.631|0.0079|-0.01

|4.00|410|0.00|5.00|35.0|7.888|7.862|7.860|6.026|0.0219|2.136|0.0988|2.256|10.280|2.400|0.000|0.907|0.607|0.0079|-0.01
|4.00|410|0.00|5.20|35.0|7.880|7.854|7.852|6.026|0.0219|2.137|0.0983|2.257|10.280|2.400|0.000|0.870|0.584|0.0079|-0.01
|4.00|410|0.00|5.40|35.0|7.871|7.845|7.844|6.026|0.0219|2.137|0.0977|2.257|10.280|2.400|0.000|0.834|0.561|0.0079|-0.01
|4.00|410|0.00|5.60|35.0|7.862|7.837|7.836|6.026|0.0219|2.138|0.0972|2.257|10.280|2.400|0.000|0.801|0.540|0.0079|-0.01
|4.00|410|0.00|5.80|35.0|7.854|7.829|7.827|6.026|0.0219|2.139|0.0966|2.258|10.280|2.400|0.000|0.769|0.520|0.0079|-0.01
|4.00|410|0.00|6.00|35.0|7.845|7.820|7.819|6.026|0.0219|2.140|0.0961|2.258|10.280|2.400|0.000|0.738|0.500|0.0079|-0.01
+----+---+----+----+----+-----+-----+-----+-----+------+-----+------+-----+------+-----+-----+-----+-----+------+