Program to derive 2D reaction phase diagrams for oxidation of SiC with ozone atom (O3)

(* R is gas constant, co2d, cod and siod are respectively the partial pressures of carbon dioxide, carbon monoxide and silicon monoxide; minT/minT2 and maxT/maxT2 are minimum and maximum temperatures and minox and maxox refer to minimum and maximum oxygen pressures*)

```
<< Graphics`

<< Graphics`MultipleListPlot`

<< Statistics`

R = 8.3143 / 1000;

cn = 2.303 * R;

co2d = -10;

cod = -10;

siod = -10;

minT = 500;

maxT = 1995;

diffT = maxT - minT;

minT2 = 2000;

maxT2 = 3200;

diffT2 = maxT2 - minT2;

minox = -50;

maxox = 1;

diffox = maxox - minox;
```

List of temperatures from 500-1995K with an increment of 5

```
Ts = Table[minT + i, {i, 0, diffT, 5}];
```

List of temperatures from 2000-3200K with an increment of 5

```
Ts2 = Table[minT2 + i, {i, 0, diffT2, 5}];
```

List of ozone partial pressures from -50 to 1 with an increment of 1

```
oxs = Table[minox + i, {i, 0, diffox, 1}];

numT = Length[Ts];

numT2 = Length[Ts2];

numox = Length[oxs];
```

List of temperatures - ozone pressures

```
Tox = Partition[Flatten[Table[{Ts[[i]], oxs[[j]]}, {i, numT}, {j, numox}]], 2];

Tox2 = Partition[Flatten[Table[{Ts2[[i]], oxs[[j]]}, {i, numT2}, {j, numox}]], 2];

Length[Tox];

Length[Tox2;]

0

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```

Reaction 1 from 298.15 – 1995 K with SiO_2 in solid phase

(* SiC+ 4/3 O_3------> SiO_2+CO_2 *);

Importing list of temperature-standard free energy of reaction values computed from program SubOXID

```
omn1 = Import["omn1", "Table"];
```

Linear regression of free energy values and temperature

```
Regress[omn1, {1, t}, t];
```

Linear regression equation

```
jk1 = Fit[omn1, {1, t}, t];
```

*Values of free energy for temperatures from 500-1995 at intervals of 5, derived from the equation *

```
tg1 = Table[jk1, {t, 500, 1995, 5}];
```

Free energy change of reaction for each temperature and ozone pressure

```
ΔGT1 = Table[tg1[[tt]] + cn * Ts[[tt]] * co2d - 4 / 3 * cn * Ts[[tt]] * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk1 = Flatten[Table[ΔGT1]];
```

Positive values of free energy change of reaction rejected (by assigning value 1000

```
Fren1 = Table[If[Frenrk1[[i]] < 0, Frenrk1[[i]], 1000], {i, 1, Length[Frenrk1]}];

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```

Reaction 1 from 2000 – 3200 K with SiO_2 in liquid phase

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(* SiC+ 4/3 O_3------> SiO_2 (liq) +CO_2 *);

Importing list of temperature-standard free energy of reaction computed from program SubOXID

```
omn13 = Import["omn13", "Table"] ;

Regress[omn13, {1, t2}, t2];

jk13 = Fit[omn13, {1, t2}, t2];

tg13 = Table[jk13, {t2, 2000, 3200, 5}];

ΔGT13 = Table[tg13[[tt2]] + cn * Ts2[[tt2]] * co2d - 4 / 3 * cn * Ts2[[tt2]] * oxs[[jj]],
   {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk13 = Flatten[Table[ΔGT13]];

Fren13 = Table[If[Frenrk13[[i]] < 0, Frenrk13[[i]], 1000], {i, 1, Length[Frenrk13]}];

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```

2 Reaction 2 from 298.15 – 1995 K with SiO2 in solid phase

(* SiC + 2/3 O_3------> SiO + CO *);

```
omn2 = Import["omn2", "Table"];
```

```
Regress[omn2, {1, t}, t];

jk2 = Fit[omn2, {1, t}, t];

tg2 = Table[jk2, {t, 500, 1995, 5}];

ΔGT2 = Table[tg2[[tt]] + cn * Ts[[tt]] * cod + cn * Ts[[tt]] * siod -
    cn * Ts[[tt]] * 2 / 3 * oxs[[jj]], {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk2 = Flatten[Table[ΔGT2]];

Fren2 = Table[If[Frenrk2[[i]] < 0, Frenrk2[[i]], 1000], {i, 1, Length[Frenrk2]}];

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```

23 Reaction 23 from 2000 – 3200 Kwith SiO2 in liquid phase

* SiC + 2/3 O_3------> SiO + CO *

```
omn23 = Import["omn23", "Table"];
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn23, {1, t2}, t2];

jk23 = Fit[omn23, {1, t2}, t2];

tg23 = Table[jk23, {t2, 2000, 3200, 5}];

ΔGT23 = Table[tg23[[tt2]] + cn * Ts2[[tt2]] * cod + cn * Ts2[[tt2]] * siod -
    cn * Ts2[[tt2]] * 2 / 3 * oxs[[jj]], {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk23 = Flatten[Table[ΔGT23]];

Fren23 = Table[If[Frenrk23[[i]] < 0, Frenrk23[[i]], 1000], {i, 1, Length[Frenrk23]}];

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```

3 Reaction 3 from 298.15 – 1995 K with SiO_2 in solid phase

(*   SiC+ O_3------> SiO_2+ CO   *);

```
omn3 = Import["omn3", "Table"] ;
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn3, {1, t}, t];
```

```
jk3 = Fit[omn3, {1, t}, t];

tg3 = Table[jk3, {t, 500, 1995, 5}];

ΔGT3 = Table[tg3[[tt]] + cn * Ts[[tt]] * cod - cn * Ts[[tt]] * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk3 = Flatten[Table[ΔGT3]];

Fren3 = Table[If[Frenrk3[[i]] < 0, Frenrk3[[i]], 1000], {i, 1, Length[Frenrk3]}];

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```

33 Reaction 3 from 2000 – 3200 K with SiO_2 in liquid phase

(* SiC+ O_3------> SiO_2+ CO *)

```
omn33 = Import["omn33", "Table"] ;
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn33, {1, t2}, t2];

jk33 = Fit[omn33, {1, t2}, t2];

tg33 = Table[jk33, {t2, 2000, 3200, 5}];

ΔGT33 = Table[tg33[[tt2]] + cn * Ts2[[tt2]] * cod - cn * Ts2[[tt2]] * oxs[[jj]],
   {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk33 = Flatten[Table[ΔGT33]];

Fren33 = Table[If[Frenrk33[[i]] < 0, Frenrk33[[i]], 1000], {i, 1, Length[Frenrk33]}];

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```

4 Reaction 4 from 298.15 – 1995 K with SiO_2 in solid phase

(* SiC + 2/3 O_3------> SiO_2 + C *);

```
omn4 = Import["omn4", "Table"];
(* Importing the values of free energy at
  different temp (upto 1800 k from 298 k) *)

Regress[omn4, {1, t}, t];

jk4 = Fit[omn4, {1, t}, t];

tg4 = Table[jk4, {t, 500, 1995, 5}];

ΔGT4 = Table[tg4[[tt]] - cn * Ts[[tt]] * 2 / 3 * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Length[ΔGT4];

Frenrk4 = Flatten[Table[ΔGT4]];

Length[Frenrk4];

Fren4 = Table[If[Frenrk4[[i]] < 0, Frenrk4[[i]], 1000], {i, 1, Length[Frenrk4]}];

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```

43 Reaction 4 from 2000 – 3200 K with SiO_2 in liquid phase

```
(*  SiC + 2/3 O3------>
  SiO2 (liq)+ C  *);

omn43 = Import["omn43", "Table"] ;
(* Importing the values of free energy
  at different temp (upto 1800 k from 298 k) *)

Regress[omn43, {1, t2}, t2];

jk43 = Fit[omn4, {1, t2}, t2];

tg43 = Table[jk43, {t2, 2000, 3200, 5}];

ΔGT43 = Table[tg43[[tt2]] - cn * Ts2[[tt2]] * 2 / 3 * oxs[[jj]],
   {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk43 = Flatten[Table[ΔGT43]];

Fren43 = Table[If[Frenrk43[[i]] < 0, Frenrk43[[i]], 1000], {i, 1, Length[Frenrk43]}];

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```

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Reaction 5 from 1298.15 – 1995 K

(* SiC+ O_3------>
SiO + CO_2 *);

```
omn5 = Import["omn5", "Table"] ;
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn5, {1, t}, t];

jk5 = Fit[omn5, {1, t}, t];

tg5 = Table[jk5, {t, 500, 1995, 5}];

ΔGT5 = Table[tg5[[tt]] + cn * Ts[[tt]] * co2d + cn * Ts[[tt]] * siod - cn * Ts[[tt]] * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk5 = Flatten[Table[ΔGT5]];

Fren5 = Table[If[Frenrk5[[i]] < 0, Frenrk5[[i]], 1000], {i, 1, Length[Frenrk5]}];

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```

53 Reaction 5 from 2000 – 3200 K

(* SiC+ O_3------>
SiO + CO_2 *);

```
omn53 = Import["omn53", "Table"];
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn53, {1, t2}, t2];

jk53 = Fit[omn53, {1, t2}, t2];

tg53 = Table[jk53, {t2, 2000, 3200, 5}];

ΔGT53 = Table[tg53[[tt2]] + cn * Ts2[[tt2]] * co2d + cn * Ts2[[tt2]] * siod -
    cn * Ts2[[tt2]] * oxs[[jj]], {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk53 = Flatten[Table[ΔGT53]];

Fren53 = Table[If[Frenrk53[[i]] < 0, Frenrk53[[i]], 1000], {i, 1, Length[Frenrk53]}];
```

```
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```

6 Reaction 6 from 298.15 – 1995 K

```
(*  SiC + 1/3 O3------>
  SiO + C  *);

omn6 = Import["omn6", "Table"] ;
(* Importing the values of free energy at
  different temp (upto 1800 k from 298 k) *)

Regress[omn6, {1, t}, t];

jk6 = Fit[omn6, {1, t}, t];

tg6 = Table[jk6, {t, 500, 1995, 5}];

ΔGT6 = Table[tg6[[tt]] + cn * Ts[[tt]] * siod - cn * Ts[[tt]] * 1 / 3 * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk6 = Flatten[Table[ΔGT6]];

Fren6 = Table[If[Frenrk6[[i]] < 0, Frenrk6[[i]], 1000], {i, 1, Length[Frenrk6]}];

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```

63 Reaction 6 from 2000 – 3200 K

```
(*  SiC + 1/3 O3------>
 SiO + C  *)

omn63 = Import["omn63", "Table"];
(* Importing the values of free energy
  at different temp (upto 1800 k from 298 k) *)

Regress[omn63, {1, t2}, t2];

jk63 = Fit[omn63, {1, t2}, t2];

tg63 = Table[jk63, {t2, 2000, 3200, 5}];

ΔGT63 = Table[tg63[[tt2]] + cn * Ts2[[tt2]] * siod - cn * Ts2[[tt2]] * 1 / 3 * oxs[[jj]],
   {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk63 = Flatten[Table[ΔGT63]];
```

```
Fren63 = Table[If[Frenrk63[[i]] < 0, Frenrk63[[i]], 1000], {i, 1, Length[Frenrk63]}];

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```

Reaction 7 from 298.15 – 1995 K

(* SiC + 2/3 O_3------> Si + CO_2 *);

```
omn7 = Import["omn7", "Table"];
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn7, {1, t}, t];

jk7 = Fit[omn7, {1, t}, t];

tg7 = Table[jk7, {t, 500, 1995, 5}];

ΔGT7 = Table[tg7[[tt]] + cn * Ts[[tt]] * co2d - cn * Ts[[tt]] * 2 / 3 * oxs[[jj]],
  {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk7 = Flatten[Table[ΔGT7]];

Fren7 = Table[If[Frenrk7[[i]] < 0, Frenrk7[[i]], 1000], {i, 1, Length[Frenrk7]}];

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```

Reaction 73 from 2000 – 3200 K

(* SiC + 2/3 O_3------> Si + CO_2 *);

```
omn73 = Import["omn73", "Table"] ;
```

(* Importing the values of free energy at different temp (upto 1800 k from 298 k) *)

```
Regress[omn73, {1, t2}, t2];

jk73 = Fit[omn73, {1, t2}, t2];

tg73 = Table[jk73, {t2, 2000, 3200, 5}];

ΔGT73 = Table[tg73[[tt2]] + cn * Ts2[[tt2]] * co2d - cn * Ts2[[tt2]] * 2 / 3 * oxs[[jj]],
  {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk73 = Flatten[Table[ΔGT73]];

Fren73 = Table[If[Frenrk73[[i]] < 0, Frenrk73[[i]], 1000], {i, 1, Length[Frenrk73]}];
```

```
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```

Reaction 8 from 298.15 – 1995 K

```
(*  SiC + 1/3 O3------>
  Si + CO  *);

omn8 = Import["omn8", "Table"];
(* Importing the values of free energy at
  different temp (upto 1800 k from 298 k) *)

Regress[omn8, {1, t}, t];

jk8 = Fit[omn8, {1, t}, t];

tg8 = Table[jk8, {t, 500, 1995, 5}];

ΔGT8 = Table[tg8[[tt]] + cn * Ts[[tt]] * cod - cn * Ts[[tt]] * 1 / 3 * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk8 = Flatten[Table[ΔGT8]];

Fren8 = Table[If[Frenrk8[[i]] < 0, Frenrk8[[i]], 1000], {i, 1, Length[Frenrk8]}];

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```

Reaction 83 from 2000 – 3200 K

```
(*  SiC + 1/3 O3------>
  Si + CO  *);

omn83 = Import["omn83", "Table"];
(* Importing the values of free energy
  at different temp (upto 1800 k from 298 k) *)

Regress[omn83, {1, t2}, t2];

jk83 = Fit[omn83, {1, t2}, t2];

tg83 = Table[jk83, {t2, 2000, 3200, 5}];

ΔGT83 = Table[tg83[[tt2]] + cn * Ts2[[tt2]] * cod - cn * Ts2[[tt2]] * 1 / 3 * oxs[[jj]],
   {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk83 = Flatten[Table[ΔGT83]];

Fren83 = Table[If[Frenrk83[[i]] < 0, Frenrk83[[i]], 1000], {i, 1, Length[Frenrk83]}];
```

```
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```

9 Reaction 9 from 298.15-1995 K

(* SiC --------> Si+ C *);

```
sds14 = Import["sds14", "Table"];
(* Importing the values of free energy
  at different temp (upto 1800 k from 298 k) *)

Regress[sds14, {1, t}, t];

jk14 = Fit[sds14, {1, t}, t];

tg14 = Table[jk14, {t, 500, 1995, 5}];

ΔGT14 = Table[tg14[[tt]] - cn * Ts[[tt]] * 0 * oxs[[jj]],
   {tt, 1, Length[Ts]}, {jj, 1, Length[oxs]}];

Frenrk14 = Flatten[Table[ΔGT14]];

Fren14 = Table[If[Frenrk14[[i]] < 0, Frenrk14[[i]], 1000], {i, 1, Length[Frenrk14]}];

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```

93 Reaction 9 from 2000-3200 K

(* Si+ C --------> SiC *);

```
sds143 = Import["sds143", "Table"];
(* Importing the values of free energy
  at different temp (upto 1800 k from 298 k) *)

Regress[sds143, {1, t2}, t2];

jk143 = Fit[sds143, {1, t2}, t2];

tg143 = Table[jk143, {t2, 2000, 3200, 5}];

ΔGT143 = Table[tg143[[tt2]] - cn * Ts2[[tt2]] * 0 * oxs[[jj]],
   {tt2, 1, Length[Ts2]}, {jj, 1, Length[oxs]}];

Frenrk143 = Flatten[Table[ΔGT143]];
```

```
Fren143 =
  Table[If[Frenrk143[[i]] < 0, Frenrk143[[i]], 1000], {i, 1, Length[Frenrk143]}];

Length[Fren143];
```

****

****

Values of free energy of reactions are compared to identify the reaction with most negative value (500-1995 K)

Make a list of free energy change for all reactions, at each value of temperature and ozone pressure

```
Do[cop[hhh] = {
   Join[{Fren1[[hhh]]}, {Fren2[[hhh]]}, {Fren3[[hhh]]},
    {Fren4[[hhh]]}, {Fren5[[hhh]]}, {Fren6[[hhh]]}, {Fren7[[hhh]]},
    {Fren8[[hhh]]}, {Fren14[[hhh]]}]}, {hhh, 1, Length[Tox]}]
```

Find the minimum value of free energy change

```
Do[mn[kkk] = {
   Min[cop[kkk]]},
           {kkk, 1, Length[Tox]}]

uy = Table[mn[kkk][[1]], {kkk, 1, Length[Tox]}];
```

Neglect positive values of free energy change (1000) by substituting with a string

```
amb = Table[If[uy[[hhh]] > 999, org, uy[[hhh]]], {hhh, 1, Length[Tox]}];
```

*** Identify which reaction gives the minimum free energy in above list ***

```
ppp = Table[Position[cop[hhh][[1]], amb[[hhh]]], {hhh, 1, Length[Tox]}];
```

*** Identify occurrences of reaction 1 from above list ***

```
sic1 = Table[Position[ppp, {{1}}]]; si1 = Flatten[sic1];
```

*** Identify the temperature and oxygen pressure corresponding to each occurrence of reaction 1 ***

```
pos1 = Table[Tox[[si1[[i]]]], {i, Length[si1]}];
```

*** Identify occurrences of reaction 2 from above list ***

```
sic2 = Table[Position[ppp, {{2}}]]; sio2 = Flatten[sic2];
```

*** Identify the temperature and oxygen pressure corresponding to each occurrence of reaction 2 ***

```
pos2 = Table[Tox[[sio2[[i]]]], {i, Length[sio2]}];
```

*** Identify occurrences of reaction 3 from above list ***

```
sic3 = Table[Position[ppp, {{3}}]]; sio3 = Flatten[sic3];
```

* Identify the temperature and oxygen pressure corresponding to each occurrence of reaction 3 *

```
pos3 = Table[Tox[[sio3[[i]]]], {i, Length[sio3]}];
```

* Identify occurrences of reaction 4 from above list *

```
sic4 = Table[Position[ppp, {{4}}]]; sio4 = Flatten[sic4];
```

* Identify the temperature and ozone pressure corresponding to each occurrence of reaction 4 *

```
pos4 = Table[Tox[[sio4[[i]]]], {i, Length[sio4]}];
```

* Identify occurrences of reaction 5 from above list *

```
sic5 = Table[Position[ppp, {{5}}]]; sio5 = Flatten[sic5];
```

* Identify the temperature and ozone pressure corresponding to each occurrence of reaction 5 *

```
pos5 = Table[Tox[[sio5[[i]]]], {i, Length[sio5]}];
```

* Identify occurrences of reaction 6 from above list *

```
sic6 = Table[Position[ppp, {{6}}]]; sio6 = Flatten[sic6];
```

* Identify the temperature and ozone pressure corresponding to each occurrence of reaction 6 *

```
pos6 = Table[Tox[[sio6[[i]]]], {i, Length[sio6]}];
```

* Identify occurrences of reaction 7 from above list *

```
sic7 = Table[Position[ppp, {{7}}]]; sio7 = Flatten[sic7];
```

* Identify the temperature and ozone pressure corresponding to each occurrence of reaction 7 *

```
pos7 = Table[Tox[[sio7[[i]]]], {i, Length[sio7]}];
```

* Identify occurrences of reaction 8 from above list *

```
sic8 = Table[Position[ppp, {{8}}]]; sio8 = Flatten[sic8];
```

* Identify the temperature and ozone pressure corresponding to each occurrence of reaction 8 *

```
pos8 = Table[Tox[[sio8[[i]]]], {i, Length[sio8]}];
```

* Identify occurrences of reaction 9 from above list *

```
sic9 = Table[Position[ppp, {{9}}]]; sio9 = Flatten[sic9];
```

* Identify the temperature and ozone pressure corresponding to each occurrence of reaction 9 *

```
pos9 = Table[Tox[[sio9[[i]]]], {i, Length[sio9]}];
```

****

****

Values of free energy of reactions are compared to identify the reaction with most negative value (2000-3200 K)

Explanatory notes as in section above

```
Do[coh2[hhh2] = {
   Join[{Fren13[[hhh2]]}, {Fren23[[hhh2]]}, {Fren33[[hhh2]]},
    {Fren43[[hhh2]]}, {Fren53[[hhh2]]}, {Fren63[[hhh2]]}, {Fren73[[hhh2]]},
    {Fren83[[hhh2]]}, {Fren143[[hhh2]]}]}, {hhh2, 1, Length[Tox2]}]

Do[mn[kkk2] = {
   Min[coh2[kkk2]]},
           {kkk2, 1, Length[Tox2]}]

tt2 = Table[mn[kkk2][[1]], {kkk2, 1, Length[Tox2]}];

amb2 = Table[If[tt2[[hhh2]] > 999, org, tt2[[hhh2]]], {hhh2, 1, Length[Tox2]}];

ppp2 = Table[Position[coh2[hhh2][[1]], amb2[[hhh2]]], {hhh2, 1, Length[Tox2]}];

sic11 = Table[Position[ppp2, {{1}}]]; si11 = Flatten[sic11];

pos11 = Table[Tox2[[si11[[i]]]], {i, Length[si11]}];

sic21 = Table[Position[ppp2, {{2}}]]; sio21 = Flatten[sic21];

pos21 = Table[Tox2[[sio21[[i]]]], {i, Length[sio21]}];

sic31 = Table[Position[ppp2, {{3}}]]; sio31 = Flatten[sic31];

pos31 = Table[Tox2[[sio31[[i]]]], {i, Length[sio31]}];
```

```
sic41 = Table[Position[ppp2, {{4}}]]; sio41 = Flatten[sic41];
pos41 = Table[Tox2[[sio41[[i]]]], {i, Length[sio41]}];
sic51 = Table[Position[ppp2, {{5}}]]; sio51 = Flatten[sic51];
pos51 = Table[Tox2[[sio51[[i]]]], {i, Length[sio51]}];
sic61 = Table[Position[ppp2, {{6}}]]; sio61 = Flatten[sic61];
pos61 = Table[Tox2[[sio61[[i]]]], {i, Length[sio61]}];
sic71 = Table[Position[ppp2, {{7}}]]; sio71 = Flatten[sic71];
pos71 = Table[Tox2[[sio71[[i]]]], {i, Length[sio71]}];
sic81 = Table[Position[ppp2, {{8}}]]; sio81 = Flatten[sic81];
pos81 = Table[Tox2[[sio81[[i]]]], {i, Length[sio81]}];
sic91 = Table[Position[ppp2, {{9}}]]; sio91 = Flatten[sic91];
pos91 = Table[Tox2[[sio91[[i]]]], {i, Length[sio91]}];
```

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Plot regions for each reaction (500-1995 K)

****

Plot regions for reaction 1

```
ListPlot[pos1]
```

****

****

Plot regions for reaction 2

```
ListPlot[pos2]
```

****

****

Plot regions for reaction 3

```
ListPlot[pos3]
```

****

****

Plot regions for reaction 4

```
ListPlot[pos4]
```

****

****

Plot regions for reaction 5

```
ListPlot[pos5]
```

****

****

Plot regions for reaction 6

```
ListPlot[pos6]
```

****

****

Plot regions for reaction 7

```
ListPlot[pos7]
```

****

****

Plot regions for reaction 8

```
ListPlot[pos8]
```

****

****

Plot regions for reaction 9

```
ListPlot[pos9]
```

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

Plot regions for each reaction (2000-3200 K)

****

****

Plot regions for reaction 1

```
ListPlot[pos11]
```

****

****

Plot regions for reaction 2

```
ListPlot[pos21]
```

****

****

Plot regions for reaction 3

```
ListPlot[pos31]
```

****

****

Plot regions for reaction 4

```
ListPlot[pos41]
```

****

****

Plot regions for reaction 5

```
ListPlot[pos51]
```

****

****

Plot regions for reaction 6

```
ListPlot[pos61]
```

****

****

Plot regions for reaction 7

```
ListPlot[pos71]
```

****

****

Plot regions for reaction 8

```
ListPlot[pos81]
```

****

****

Plot regions for reaction 9

```
ListPlot[pos91]
```

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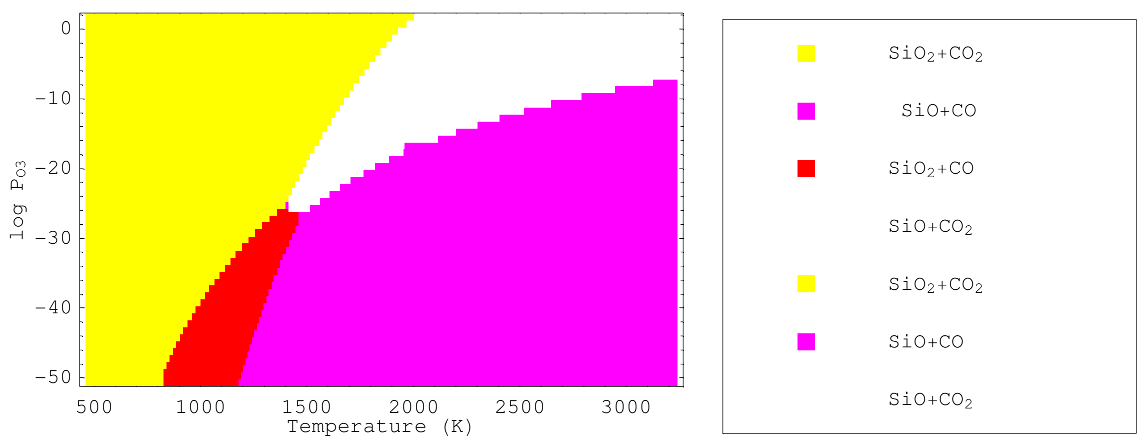
Combining all plots into a single 2D colour graphics

```
plot2dozone = MultipleListPlot[pos1, pos2, pos3, pos5, pos11, pos21, pos51,
  SymbolShape → {PlotSymbol[Box, 4], PlotSymbol[Box, 4], PlotSymbol[Box, 4],
    PlotSymbol[Box, 4], PlotSymbol[Box, 4], PlotSymbol[Box, 4], PlotSymbol[Box, 4]},
  SymbolStyle → {RGBColor[1, 1, 0], RGBColor[1, 0, 1], RGBColor[1, 0, 0],
    RGBColor[1, 1, 1], RGBColor[1, 1, 0], RGBColor[1, 0, 1], RGBColor[1, 1, 1]},
  Frame → True, PlotLegend → {"SiO2+CO2", " SiO+CO", "SiO2+CO", "SiO+CO2",
    "SiO2+CO2", "SiO+CO", "SiO+CO2"}, LegendSize → {1.2, 1.2},
  FrameLabel → {"Temperature (K)", "log PO3"}, PlotRange → All]
```



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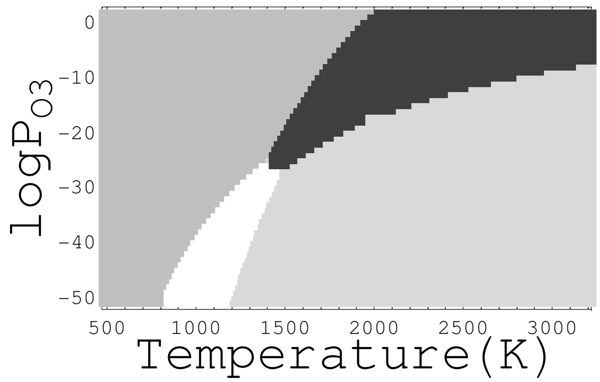
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

Grey scale representation of the above figure

```
plot2dozone10 = MultipleListPlot[pos1, pos2, pos3, pos5, pos11, pos21, pos51,
  SymbolShape → {PlotSymbol[Box, 4], PlotSymbol[Box, 4], PlotSymbol[Box, 4],
    PlotSymbol[Box, 4], PlotSymbol[Box, 4], PlotSymbol[Box, 4], PlotSymbol[Box, 4]},
  SymbolStyle → {GrayLevel[0.75], GrayLevel[0.85], GrayLevel[1], GrayLevel[0.25],
    GrayLevel[0.75], GrayLevel[0.85], GrayLevel[0.25]}, Frame → True,
  FrameLabel → {"Temperature(K) ", "logPO3"},
  PlotRange → {{minT - 30, maxT2 + 20}, {minox - 2, maxox + 2}}]
```



Export to other formats

```
Export["plot2dozone10.eps", plot2dozone10, ImageSize -> {400, 400}];

Export["plot2dozone10.tif", plot2dozone10, ImageSize -> {400, 400}];

Export["plot2dozone10.bmp", plot2dozone10, ImageSize -> {400, 400}];
```