Program to calculate standard free energy change, equilibrium constant and equilibrium ozone pressure of SiC oxidation reactions with ozone (O3) at temperatures from 2000 to 3200 K

##

##########################

* Constants*

```
R = 8.3143 / 1000;

co2d = 0;

cod = 0;

siod = 0;
```

- *** Input data from thermodynamic tables : Temperatures and corresponding standard free energies of formation (dg) of the compounds***

```
(*  SiC  *)

temp3 = {2000, 2100, 2200, 2300, 2400, 2500, 2600, 2700, 2800, 2900, 3000, 3100, 3200};

dg_sic3 = {-48.450, -44.738, -41.034, -37.338, -33.649,
   -29.967, -26.294, -22.627, -18.967, -15.315, -11.669, -8.030, -4.397};

dg_sio23 = {-551.112, -531.950, -512.900, -493.93, -475.047, -456.253,
   -437.529, -418.894, \-400.321, -381.807, -363.376, -344.996, -326.678};

dg_co23 = {-396.442, -396.417, -396.409, -396.371, -396.325, -396.283,
   -396.216, -396.\154, -396.066, -395.97, -395.869, -395.752, -395.639};

dg_sio3 = {-256.651, -261.228, -265.776, -270.278, -274.726, -279.161,
   -283.541, -287.\888, -292.206, -296.482, -300.738, -304.955, -309.152};

dg_co3 = {-285.989, -294.328, -302.65, -310.917, -319.164, -327.385,
   -335.565, -343.728, -351.845, -359.941, -368.012, -376.05, -384.07};
```

```
dg_cgr3 = 0;

dg_si3 = 0;

caldg_O33 = {66.680, 68.272, 69.861, 71.449, 73.039,
   74.623, 76.211, 77.797, 79.383, 80.971, 82.557, 84.145, 85.731};

dg_O33 = 4.184 * caldg_O33;
```

$$13$$

(* SiC+ 4/3 O3------> SiO_2 (liq)+CO_2 *)

- *** Standard free energy change of reaction 13 (G13)**

```
G13 = (dg_sio23 + dg_co23 - dg_sic3 - 4 / 3 * dg_O33);
```

- *** Temperature - Equilibrium oxygen activity list for reaction '13' (eqbs13)**

```
a13 = (3 * G13 / (4 * R * temp3 * 2.303)) + 3 / 4 * co2d;

ozlw013 = {{temp3[[1]], a13[[1]]}, {temp3[[2]], a13[[2]]},
   {temp3[[3]], a13[[3]]}, {temp3[[4]], a13[[4]]}, {temp3[[5]], a13[[5]]},
   {temp3[[6]], a13[[6]]}, {temp3[[7]], a13[[7]]}, {temp3[[8]], a13[[8]]},
   {temp3[[9]], a13[[9]]}, {temp3[[10]], a13[[10]]}, {temp3[[11]], a13[[11]]},
   {temp3[[12]], a13[[12]]}, {temp3[[13]], a13[[13]]}};
```

- *** Plot of Temperature - Equilibrium oxygen activity list for reaction 13***

```
ListPlot[ozlw013]
```

- *** Export data***

```
Export["ozlw013", ozlw013, "Table"];
```

- *** List of Temperature-Standard free energy change of reaction 13**

```
omn13 = {{temp3[[1]], G13[[1]]}, {temp3[[2]], G13[[2]]},
   {temp3[[3]], G13[[3]]}, {temp3[[4]], G13[[4]]}, {temp3[[5]], G13[[5]]},
   {temp3[[6]], G13[[6]]}, {temp3[[7]], G13[[7]]}, {temp3[[8]], G13[[8]]},
   {temp3[[9]], G13[[9]]}, {temp3[[10]], G13[[10]]}, {temp3[[11]], G13[[11]]},
   {temp3[[12]], G13[[12]]}, {temp3[[13]], G13[[13]]}};
```

- *** Plot of Temperature-Standard free energy change of reaction 13***

```
ListPlot[omn13]
```

* Export list of Temperature-Standard free energy change of reaction 13*

```
Export["omn13", omn13, "Table"];
```

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```
         2 3
(*   SiC  +  2/3 O3------->  SiO  +  CO    *) ;
```

* Standard free energy change of reaction 23 (G23)

```
G23 = (dgsio3 + dgco3 - dgsic3 - 2 / 3 * dgo33) ;
```

* Equilibrium oxygen activity for reaction 23 (a23)

```
a23 = (3 * G23 / (2 * R * temp3 * 2.303)) + 3 / 2 * cod + 3 / 2 * siod;
```

* Temperature - Equilibrium oxygen activity list for reaction 23 (eqbs23)

```
ozlw023 = {{temp3[[1]], a23[[1]]}, {temp3[[2]], a23[[2]]},
   {temp3[[3]], a23[[3]]}, {temp3[[4]], a23[[4]]}, {temp3[[5]], a23[[5]]},
   {temp3[[6]], a23[[6]]}, {temp3[[7]], a23[[7]]}, {temp3[[8]], a23[[8]]},
   {temp3[[9]], a23[[9]]}, {temp3[[10]], a23[[10]]}, {temp3[[11]], a23[[11]]},
   {temp3[[12]], a23[[12]]}, {temp3[[13]], a23[[13]]}};
```

* Plot of Temperature-Standard free energy change of reaction 23*

```
ListPlot[ozlw023]
```

* Export data*

```
Export["ozlw023", ozlw023, "Table"];
```

* List of Temperature-Standard free energy change of reaction 23

```
omn23 = {{temp3[[1]], G23[[1]]}, {temp3[[2]], G23[[2]]},
   {temp3[[3]], G23[[3]]}, {temp3[[4]], G23[[4]]}, {temp3[[5]], G23[[5]]},
   {temp3[[6]], G23[[6]]}, {temp3[[7]], G23[[7]]}, {temp3[[8]], G23[[8]]},
   {temp3[[9]], G23[[9]]}, {temp3[[10]], G23[[10]]}, {temp3[[11]], G23[[11]]},
   {temp3[[12]], G23[[12]]}, {temp3[[13]], G23[[13]]}};
```

* Plot of Temperature-Standard free energy change of reaction 2*

```
ListPlot[omn23]
```

■ * Export list of Temperature-Standard free energy change of reaction 2*

```
Export["omn23", omn23, "Table"];
```

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33

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

■ * Standard free energy change of reaction 33 (G33)

$$G33 = (dg_{sio23} + dg_{co3} - dg_{sic3} - dg_{O33});$$

■ * Equilibrium oxygen activity for reaction 33 (a33)

```
a33 = (G33 / (R * temp3 * 2.303)) + cod;
```

■ * Temperature - Equilibrium oxygen activity list for reaction 33 (eqbs33)

```
ozlw033 = {{temp3[[1]], a33[[1]]}, {temp3[[2]], a33[[2]]},
   {temp3[[3]], a33[[3]]}, {temp3[[4]], a33[[4]]}, {temp3[[5]], a33[[5]]},
   {temp3[[6]], a33[[6]]}, {temp3[[7]], a33[[7]]}, {temp3[[8]], a33[[8]]},
   {temp3[[9]], a33[[9]]}, {temp3[[10]], a33[[10]]}, {temp3[[11]], a33[[11]]},
   {temp3[[12]], a33[[12]]}, {temp3[[13]], a33[[13]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 33*

```
ListPlot[ozlw033]
```

■ * Export data*

```
Export["ozlw033", ozlw033, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 33

```
omn33 = {{temp3[[1]], G33[[1]]}, {temp3[[2]], G33[[2]]},
   {temp3[[3]], G33[[3]]}, {temp3[[4]], G33[[4]]}, {temp3[[5]], G33[[5]]},
   {temp3[[6]], G33[[6]]}, {temp3[[7]], G33[[7]]}, {temp3[[8]], G33[[8]]},
   {temp3[[9]], G33[[9]]}, {temp3[[10]], G33[[10]]}, {temp3[[11]], G33[[11]]},
   {temp3[[12]], G33[[12]]}, {temp3[[13]], G33[[13]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 33*

```
ListPlot[omn33]
```

■ * Export list of Temperature-Standard free energy change of reaction 33*

```
Export["omn33", omn33, "Table"];
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43

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

■ * Standard free energy change of reaction 43 (G43)

$$G43 = (dg_{sio23} + dg_{cgr3} - dg_{sic3} - 2/3 * dg_{O33});$$

■ * Equilibrium oxygen activity for reaction 43 (a43)

```
a43 = (3 * G43) / (2 * R * temp3 * 2.303);
```

■ * Temperature - Equilibrium oxygen activity list for reaction 43 (eqbs43)

```
ozlw043 = {{temp3[[1]], a43[[1]]}, {temp3[[2]], a43[[2]]},
   {temp3[[3]], a43[[3]]}, {temp3[[4]], a43[[4]]}, {temp3[[5]], a43[[5]]},
   {temp3[[6]], a43[[6]]}, {temp3[[7]], a43[[7]]}, {temp3[[8]], a43[[8]]},
   {temp3[[9]], a43[[9]]}, {temp3[[10]], a43[[10]]}, {temp3[[11]], a43[[11]]},
   {temp3[[12]], a43[[12]]}, {temp3[[13]], a43[[13]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 43*

```
ListPlot[ozlw043]
```

■ * Export data*

```
Export["ozlw043", ozlw043, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 43

```
omn43 = {{temp3[[1]], G43[[1]]}, {temp3[[2]], G43[[2]]},
   {temp3[[3]], G43[[3]]}, {temp3[[4]], G43[[4]]}, {temp3[[5]], G43[[5]]},
   {temp3[[6]], G43[[6]]}, {temp3[[7]], G43[[7]]}, {temp3[[8]], G43[[8]]},
   {temp3[[9]], G43[[9]]}, {temp3[[10]], G43[[10]]}, {temp3[[11]], G43[[11]]},
   {temp3[[12]], G43[[12]]}, {temp3[[13]], G43[[13]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 43*

```
ListPlot[omn43]
```

* Export list of Temperature-Standard free energy change of reaction 43*

```
Export["omn43", omn43, "Table"];
```

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```

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

* Standard free energy change of reaction 53 (G53)

$$G53 = (dg_{sio3} + dg_{co23} - dg_{sic3} - dg_{o33}) \;;$$

* Equilibrium oxygen activity for reaction 53 (a53)

```
a53 = (G53) / (R * temp3 * 2.303) + co2d + siod;
```

* Temperature - Equilibrium oxygen activity list for reaction 53 (eqbs53)

```
ozlw053 = {{temp3[[1]], a53[[1]]}, {temp3[[2]], a53[[2]]},
   {temp3[[3]], a53[[3]]}, {temp3[[4]], a53[[4]]}, {temp3[[5]], a53[[5]]},
   {temp3[[6]], a53[[6]]}, {temp3[[7]], a53[[7]]}, {temp3[[8]], a53[[8]]},
   {temp3[[9]], a53[[9]]}, {temp3[[10]], a53[[10]]}, {temp3[[11]], a53[[11]]},
   {temp3[[12]], a53[[12]]}, {temp3[[13]], a53[[13]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 53*

```
ListPlot[ozlw053]
```

* Export data*

```
Export["ozlw053", ozlw053, "Table"];
```

* List of Temperature-Standard free energy change of reaction 53

```
omn53 = {{temp3[[1]], G53[[1]]}, {temp3[[2]], G53[[2]]},
   {temp3[[3]], G53[[3]]}, {temp3[[4]], G53[[4]]}, {temp3[[5]], G53[[5]]},
   {temp3[[6]], G53[[6]]}, {temp3[[7]], G53[[7]]}, {temp3[[8]], G53[[8]]},
   {temp3[[9]], G53[[9]]}, {temp3[[10]], G53[[10]]}, {temp3[[11]], G53[[11]]},
   {temp3[[12]], G53[[12]]}, {temp3[[13]], G53[[13]]}};
```

* Plot of Temperature-Standard free energy change of reaction 53*

```
ListPlot[omn53]
```

■ *** Export list of Temperature-Standard free energy change of reaction 53***

```
Export["omn53", omn53, "Table"];
```

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```
          63
(*   SiC + 1/3 O3------> SiO + C   *) ;
```

■ *** Standard free energy change of reaction 63 (G63)**

$$G63 = (dg_{sio3} + dg_{cgr3} - dg_{sic3} - 1/3 * dg_{O33}) \quad ;$$

■ *** Equilibrium oxygen activity for reaction 63 (a63)**

```
a63 = (3 * G63) / (R * temp3 * 2.303) + 3 * siod;
```

■ *** Temperature - Equilibrium oxygen activity list for reaction 63 (eqbs63)**

```
ozlw063 = {{temp3[[1]], a63[[1]]}, {temp3[[2]], a63[[2]]},
   {temp3[[3]], a63[[3]]}, {temp3[[4]], a63[[4]]}, {temp3[[5]], a63[[5]]},
   {temp3[[6]], a63[[6]]}, {temp3[[7]], a63[[7]]}, {temp3[[8]], a63[[8]]},
   {temp3[[9]], a63[[9]]}, {temp3[[10]], a63[[10]]}, {temp3[[11]], a63[[11]]},
   {temp3[[12]], a63[[12]]}, {temp3[[13]], a63[[13]]}};
```

■ *** Plot of Temperature - Equilibrium oxygen activity list for reaction 63***

```
ListPlot[ozlw063]
```

■ *** Export data***

```
Export["ozlw063", ozlw063, "Table"];
```

■ *** List of Temperature-Standard free energy change of reaction 63**

```
omn63 = {{temp3[[1]], G63[[1]]}, {temp3[[2]], G63[[2]]},
   {temp3[[3]], G63[[3]]}, {temp3[[4]], G63[[4]]}, {temp3[[5]], G63[[5]]},
   {temp3[[6]], G63[[6]]}, {temp3[[7]], G63[[7]]}, {temp3[[8]], G63[[8]]},
   {temp3[[9]], G63[[9]]}, {temp3[[10]], G63[[10]]}, {temp3[[11]], G63[[11]]},
   {temp3[[12]], G63[[12]]}, {temp3[[13]], G63[[13]]}};
```

■ *** Plot of Temperature-Standard free energy change of reaction 63***

```
ListPlot[omn63]
```

■ * Export list of Temperature-Standard free energy change of reaction 63*

```
Export["omn63", omn63, "Table"];
```

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73

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

■ * Standard free energy change of reaction 73 (G73)

$$G73 = (dg_{si3} + dg_{co23} - dg_{sic3} - 2/3 * dg_{O33});$$

■ * Equilibrium oxygen activity for reaction 73 (a73)

```
a73 = (3 * G73) / (2 * R * temp3 * 2.303) + 3 / 2 * co2d;
```

■ * Temperature - Equilibrium oxygen activity list for reaction 73 (eqbs73)

```
ozlw073 = {{temp3[[1]], a73[[1]]}, {temp3[[2]], a73[[2]]},
   {temp3[[3]], a73[[3]]}, {temp3[[4]], a73[[4]]}, {temp3[[5]], a73[[5]]},
   {temp3[[6]], a73[[6]]}, {temp3[[7]], a73[[7]]}, {temp3[[8]], a73[[8]]},
   {temp3[[9]], a73[[9]]}, {temp3[[10]], a73[[10]]}, {temp3[[11]], a73[[11]]},
   {temp3[[12]], a73[[12]]}, {temp3[[13]], a73[[13]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 73*

```
ListPlot[ozlw073]
```

■ * Export data*

```
Export["ozlw073", ozlw073, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 73

```
omn73 = {{temp3[[1]], G73[[1]]}, {temp3[[2]], G73[[2]]},
   {temp3[[3]], G73[[3]]}, {temp3[[4]], G73[[4]]}, {temp3[[5]], G73[[5]]},
   {temp3[[6]], G73[[6]]}, {temp3[[7]], G73[[7]]}, {temp3[[8]], G73[[8]]},
   {temp3[[9]], G73[[9]]}, {temp3[[10]], G73[[10]]}, {temp3[[11]], G73[[11]]},
   {temp3[[12]], G73[[12]]}, {temp3[[13]], G73[[13]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 73*

```
ListPlot[omn73]
```

* Export list of Temperature-Standard free energy change of reaction 73*

```
Export["omn73", omn73, "Table"];
```

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```

83

(* SiC + 1/3 O_3------> Si + CO *);

* Standard free energy change of reaction 83 (G83)

$$G83 = (dg_{si3} + dg_{co3} - dg_{sic3} - 1/3 * dg_{O33});$$

* Equilibrium oxygen activity for reaction 83 (a83)

```
a83 = (3 * G83) / (R * temp3 * 2.303) + (cod * 3);
```

* Temperature - Equilibrium oxygen activity list for reaction 83 (eqbs83)

```
ozlw083 = {{temp3[[1]], a83[[1]]}, {temp3[[2]], a83[[2]]},
   {temp3[[3]], a83[[3]]}, {temp3[[4]], a83[[4]]}, {temp3[[5]], a83[[5]]},
   {temp3[[6]], a83[[6]]}, {temp3[[7]], a83[[7]]}, {temp3[[8]], a83[[8]]},
   {temp3[[9]], a83[[9]]}, {temp3[[10]], a83[[10]]}, {temp3[[11]], a83[[11]]},
   {temp3[[12]], a83[[12]]}, {temp3[[13]], a83[[13]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 83*

```
ListPlot[ozlw083]
```

* Export data*

```
Export["ozlw083", ozlw083, "Table"];
```

* List of Temperature-Standard free energy change of reaction 83

```
omn83 = {{temp3[[1]], G83[[1]]}, {temp3[[2]], G83[[2]]},
   {temp3[[3]], G83[[3]]}, {temp3[[4]], G83[[4]]}, {temp3[[5]], G83[[5]]},
   {temp3[[6]], G83[[6]]}, {temp3[[7]], G83[[7]]}, {temp3[[8]], G83[[8]]},
   {temp3[[9]], G83[[9]]}, {temp3[[10]], G83[[10]]}, {temp3[[11]], G83[[11]]},
   {temp3[[12]], G83[[12]]}, {temp3[[13]], G83[[13]]}};
```

* Plot of Temperature-Standard free energy change of reaction 83*

```
ListPlot[omn83]
```

* Export list of Temperature-Standard free energy change of reaction 83*

```
Export["omn83", omn83, "Table"];
```

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```
103 (* Si+1/3 O3-------> SiO *);
```

* Standard free energy change of reaction 103 (G103)

$$G103 = (dg_{sio3} - dg_{si3} - 1/3 * dg_{o33});$$

* Equilibrium oxygen activity list for reaction 103 (eqbs103)

```
a103 = (3 * G103) / (R * temp3 * 2.303) + 3 * siod;
```

* Temperature - Equilibrium oxygen activity list for reaction 103 (eqbs103)

```
ozlw0103 = {{temp3[[1]], a103[[1]]}, {temp3[[2]], a103[[2]]},
   {temp3[[3]], a103[[3]]}, {temp3[[4]], a103[[4]]}, {temp3[[5]], a103[[5]]},
   {temp3[[6]], a103[[6]]}, {temp3[[7]], a103[[7]]}, {temp3[[8]], a103[[8]]},
   {temp3[[9]], a103[[9]]}, {temp3[[10]], a103[[10]]}, {temp3[[11]], a103[[11]]},
   {temp3[[12]], a103[[12]]}, {temp3[[13]], a103[[13]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 103*

```
ListPlot[ozlw0103]
```

* Export data*

```
Export["ozlw0103", ozlw0103, "Table"];
```

* List of Temperature-Standard free energy change of reaction 103*

```
omn103 = {{temp3[[1]], G103[[1]]}, {temp3[[2]], G103[[2]]},
   {temp3[[3]], G103[[3]]}, {temp3[[4]], G103[[4]]}, {temp3[[5]], G103[[5]]},
   {temp3[[6]], G103[[6]]}, {temp3[[7]], G103[[7]]}, {temp3[[8]], G103[[8]]},
   {temp3[[9]], G103[[9]]}, {temp3[[10]], G103[[10]]}, {temp3[[11]], G103[[11]]},
   {temp3[[12]], G103[[12]]}, {temp3[[13]], G103[[13]]}};
```

* Plot of Temperature-Standard free energy change of reaction 103*

```
ListPlot[omn103]
```

■ * Export list of Temperature-Standard free energy change of reaction 103*

```
Export["omn103", omn103, "Table"];
```

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```

113 (* Si + 2/3*O_3------> SiO_2 *);

■ * Standard free energy change of reaction 11 (G11)

$$G113 = (dg_{sio23} - dg_{si3} - 2/3*dg_{O33});$$

■ * Equilibrium oxygen activity for reaction 113 (a113)

```
a113 = (3 * G113) / (2 * R * temp3 * 2.303);
```

■ * Temperature - Equilibrium oxygen activity list for reaction 113 (eqbs113)

```
ozlw0113 = {{temp3[[1]], a113[[1]]}, {temp3[[2]], a113[[2]]},
   {temp3[[3]], a113[[3]]}, {temp3[[4]], a113[[4]]}, {temp3[[5]], a113[[5]]},
   {temp3[[6]], a113[[6]]}, {temp3[[7]], a113[[7]]}, {temp3[[8]], a113[[8]]},
   {temp3[[9]], a113[[9]]}, {temp3[[10]], a113[[10]]}, {temp3[[11]], a113[[11]]},
   {temp3[[12]], a113[[12]]}, {temp3[[13]], a113[[13]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 113*

```
ListPlot[ozlw0113]
```

■ * Export data*

```
Export["ozlw0113", ozlw0113, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 113

```
omn113 = {{temp3[[1]], G113[[1]]}, {temp3[[2]], G113[[2]]},
   {temp3[[3]], G113[[3]]}, {temp3[[4]], G113[[4]]}, {temp3[[5]], G113[[5]]},
   {temp3[[6]], G113[[6]]}, {temp3[[7]], G113[[7]]}, {temp3[[8]], G113[[8]]},
   {temp3[[9]], G113[[9]]}, {temp3[[10]], G113[[10]]}, {temp3[[11]], G113[[11]]},
   {temp3[[12]], G113[[12]]}, {temp3[[13]], G113[[13]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 113*

```
ListPlot[omn113]
```

■ * Export list of Temperature-Standard free energy change of reaction 113*

```
Export["omn113", omn113, "Table"];
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143
(* Si+ C ------> SiC *);

$G143_{SiC} = dg_{sic3}$;

G143 = $G143_{SiC}$;

■ * List of Temperature-Standard free energy change of reaction 143*

```
sds143 = {{temp3[[1]], G143[[1]]}, {temp3[[2]], G143[[2]]},
   {temp3[[3]], G143[[3]]}, {temp3[[4]], G143[[4]]}, {temp3[[5]], G143[[5]]},
   {temp3[[6]], G143[[6]]}, {temp3[[7]], G143[[7]]}, {temp3[[8]], G143[[8]]},
   {temp3[[9]], G143[[9]]}, {temp3[[10]], G143[[10]]}, {temp3[[11]], G143[[11]]},
   {temp3[[12]], G143[[12]]}, {temp3[[13]], G143[[13]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 143*

```
ListPlot[sds143]
```

■ * Export list of Temperature-Standard free energy change of reaction 143*

```
Export["sds143", sds143, "Table"];
```

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* Oxidation of C*

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153 (* C + 1/3 O_3 ------> CO *);

■ * Standard free energy change of reaction 153 (G153)

G153 = $dg_{co3} - 1/3 * dg_{o33}$;

■ * Equilibrium oxygen activity for reaction 153 (a153)

```
a153 = (3 * G153) / (R * temp3 * 2.303) + (cod * 3);
```

■ * Temperature - Equilibrium oxygen activity list for reaction153 (eqbs153)

```
ozlw0153 = {{temp3[[1]], a153[[1]]}, {temp3[[2]], a153[[2]]},
   {temp3[[3]], a153[[3]]}, {temp3[[4]], a153[[4]]}, {temp3[[5]], a153[[5]]},
   {temp3[[6]], a153[[6]]}, {temp3[[7]], a153[[7]]}, {temp3[[8]], a153[[8]]},
   {temp3[[9]], a153[[9]]}, {temp3[[10]], a153[[10]]}, {temp3[[11]], a153[[11]]},
   {temp3[[12]], a153[[12]]}, {temp3[[13]], a153[[13]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 153*

```
ListPlot[ozlw0153]
```

■ * Export data*

```
Export["ozlw0153", ozlw0153, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 153*

```
omn153 = {{temp3[[1]], G153[[1]]}, {temp3[[2]], G153[[2]]},
   {temp3[[3]], G153[[3]]}, {temp3[[4]], G153[[4]]}, {temp3[[5]], G153[[5]]},
   {temp3[[6]], G153[[6]]}, {temp3[[7]], G153[[7]]}, {temp3[[8]], G153[[8]]},
   {temp3[[9]], G153[[9]]}, {temp3[[10]], G153[[10]]}, {temp3[[11]], G153[[11]]},
   {temp3[[12]], G153[[12]]}, {temp3[[13]], G153[[13]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 153

```
ListPlot[omn153]
```

■ * Export list of Temperature-Standard free energy change of reaction 153*

```
Export["omn153", omn153, "Table"];

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx\
 xxxxxxxxxx
```

163 (* $C + 2/3*O_3$ ------> CO_2 *);

■ * Standard free energy change of reaction 163 (G163)

G163 = $dg_{co23} - 2/3 * dg_{o33}$;

■ *** Equilibrium oxygen activity for reaction 163 (a163)**

```
a163 = (3 * G163 / (2 * R * temp3 * 2.303)) + 3 / 2 * co2d;
```

■ *** Temperature - Equilibrium oxygen activity list for reaction 163 (eqbs163)**

```
ozlw0163 = {{temp3[[1]], a163[[1]]}, {temp3[[2]], a163[[2]]},
   {temp3[[3]], a163[[3]]}, {temp3[[4]], a163[[4]]}, {temp3[[5]], a163[[5]]},
   {temp3[[6]], a163[[6]]}, {temp3[[7]], a163[[7]]}, {temp3[[8]], a163[[8]]},
   {temp3[[9]], a163[[9]]}, {temp3[[10]], a163[[10]]}, {temp3[[11]], a163[[11]]},
   {temp3[[12]], a163[[12]]}, {temp3[[13]], a163[[13]]}};
```

■ *** Plot of Temperature - Equilibrium oxygen activity list for reaction 163***

```
ListPlot[ozlw0163]
```

■ *** Export data***

```
Export["ozlw163", ozlw163, "Table"];
```

■ *** List of Temperature-Standard free energy change of reaction 163***

```
omn163 = {{temp3[[1]], G163[[1]]}, {temp3[[2]], G163[[2]]},
   {temp3[[3]], G163[[3]]}, {temp3[[4]], G163[[4]]}, {temp3[[5]], G163[[5]]},
   {temp3[[6]], G163[[6]]}, {temp3[[7]], G163[[7]]}, {temp3[[8]], G163[[8]]},
   {temp3[[9]], G163[[9]]}, {temp3[[10]], G163[[10]]}, {temp3[[11]], G163[[11]]},
   {temp3[[12]], G163[[12]]}, {temp3[[13]], G163[[13]]}};
```

■ ***Plot of Temperature-Standard free energy change of reaction 163***

```
ListPlot[omn163]
```

■ *** Export list of Temperature-Standard free energy change of reaction 163***

```
Export["omn163", omn163, "Table"];
```

```
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx\
 xxxxxxxxxxxxxxxx
```