* Program to calculate standard free energy change, equilibrium constant and equilibrium ozone pressure of SiC oxidation reactions with ozone (O3) at temperatures from 298.15 to 1900 K *

#

* Constants*

```
R = 8.3143 / 1000;

co2d = 0;

cod = 0;

siod = 0;

temp = {298.15, 400, 500, 600, 700, 800, 900,
   1000, 1100, 1200, 1300, 1400, 1500, 1600, 1700, 1800, 1900};

dg_sio2 = {-856.477, -837.859, -819.595, -801.433, -783.408,
   -765.542, -747.882, -730.363, -712.924, -695.552, -678.243,
   -661.018, -643.838, -626.726, -609.220, -589.245, -569.342};

dg_co2 = {-394.405, -394.698, -394.965, -395.212, -395.430,
   -395.622, -395.790, -395.924, -396.049, -396.145, -396.229,
   -396.292, -396.342, -396.388, -396.417, -396.434, -396.438};

dg_sic = {-70.85, -70.025, -69.215, -68.417, -67.633, -66.859, -66.094, -65.336, -64.583,
   -63.832, -63.048, -62.335, -61.585, -60.832, -59.629, -55.895, -52.169};

caldg_O3 = {38.997, 40.684, 42.351, 44.015, 45.672, 47.321, 48.963, 50.599,
   52.227, 53.85, 55.468, 57.08, 58.688, 60.293, 61.895, 63.492, 65.088};

dg_O3 = 4.184 * caldg_O3;

dg_co = {-137.164, -146.335, -155.410, -164.477, -173.502,
   -182.473, -191.393, -200.242, -209.041, -217.773, -226.463,
   -235.095, -243.680, -252.228, -260.726, -269.186, -277.604};

dg_sio = {-127.290, -136.386, -145.160, -153.808, -162.343,
   -170.778, -179.113, -187.368, -195.543, -203.644, -211.669,
   -219.622, -227.501, -235.325, -242.639, -247.350, -252.032};

dg_cgr = 0;
```

```
dg_si = 0;
```

(* SiC+ 4/3 O_3------> SiO_2+CO_2 *); [1]

* Standard free energy change of reaction 1 (G1)

$$G1 = (dg_{sio2} + dg_{co2} - dg_{sic} - 4 / 3 * dg_{O3});$$

* Equilibrium oxygen activity for reaction '1' (a1)

```
a1 = ((3 * G1) / (4 * R * temp * 2.303)) + (3 * co2d / 4);
```

* Temperature - Equilibrium oxygen activity list for reaction '1' (eqbs1)

```
ozlw01 = {{temp[[1]], a1[[1]]}, {temp[[2]], a1[[2]]},
   {temp[[3]], a1[[3]]}, {temp[[4]], a1[[4]]}, {temp[[5]], a1[[5]]},
   {temp[[6]], a1[[6]]}, {temp[[7]], a1[[7]]}, {temp[[8]], a1[[8]]},
   {temp[[9]], a1[[9]]}, {temp[[10]], a1[[10]]}, {temp[[11]], a1[[11]]},
   {temp[[12]], a1[[12]]}, {temp[[13]], a1[[13]]}, {temp[[14]], a1[[14]]},
   {temp[[15]], a1[[15]]}, {temp[[16]], a1[[16]]}, {temp[[17]], a1[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 1*

```
ListPlot[ozlw01]
```

* Export data*

```
Export["ozlw01", ozlw01, "Table"];
```

* List of Temperature-Standard free energy change of reaction 1

```
omn1 = {{temp[[1]], G1[[1]]}, {temp[[2]], G1[[2]]},
   {temp[[3]], G1[[3]]}, {temp[[4]], G1[[4]]}, {temp[[5]], G1[[5]]},
   {temp[[6]], G1[[6]]}, {temp[[7]], G1[[7]]}, {temp[[8]], G1[[8]]},
   {temp[[9]], G1[[9]]}, {temp[[10]], G1[[10]]}, {temp[[11]], G1[[11]]},
   {temp[[12]], G1[[12]]}, {temp[[13]], G1[[13]]}, {temp[[14]], G1[[14]]},
   {temp[[15]], G1[[15]]}, {temp[[16]], G1[[16]]}, {temp[[17]], G1[[17]]}};

ListPlot[omn1]
```

* Export list of Temperature-Standard free energy change of reaction 1*

```
Export["omn1", omn1, "Table"];

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```

$$(*\quad SiC + 2/3\, O_3 \xrightarrow{2} SiO + CO \quad *);$$

- *** Standard free energy change of reaction 2 (G2)**

$$G2 = (dg_{sio} + dg_{co} - dg_{sic} - 2 / 3 * dg_{o3});$$

- *** Equilibrium oxygen activity for reaction 2 (a2)**

```
a2 = ((3 * G2) / (2 * R * temp * 2.303)) + 3 / 2 * cod + 3 / 2 * siod;
```

- *** Temperature - Equilibrium oxygen activity list for reaction 2 (eqbs2)**

```
ozlw02 = {{temp[[1]], a2[[1]]}, {temp[[2]], a2[[2]]},
   {temp[[3]], a2[[3]]}, {temp[[4]], a2[[4]]}, {temp[[5]], a2[[5]]},
   {temp[[6]], a2[[6]]}, {temp[[7]], a2[[7]]}, {temp[[8]], a2[[8]]},
   {temp[[9]], a2[[9]]}, {temp[[10]], a2[[10]]}, {temp[[11]], a2[[11]]},
   {temp[[12]], a2[[12]]}, {temp[[13]], a2[[13]]}, {temp[[14]], a2[[14]]},
   {temp[[15]], a2[[15]]}, {temp[[16]], a2[[16]]}, {temp[[17]], a2[[17]]}};
```

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

```
ListPlot[ozlw02]
```

- *** Export data***

```
Export["ozlw02", ozlw02, "Table"];
```

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

```
omn2 = {{temp[[1]], G2[[1]]}, {temp[[2]], G2[[2]]},
   {temp[[3]], G2[[3]]}, {temp[[4]], G2[[4]]}, {temp[[5]], G2[[5]]},
   {temp[[6]], G2[[6]]}, {temp[[7]], G2[[7]]}, {temp[[8]], G2[[8]]},
   {temp[[9]], G2[[9]]}, {temp[[10]], G2[[10]]}, {temp[[11]], G2[[11]]},
   {temp[[12]], G2[[12]]}, {temp[[13]], G2[[13]]}, {temp[[14]], G2[[14]]},
   {temp[[15]], G2[[15]]}, {temp[[16]], G2[[16]]}, {temp[[17]], G2[[17]]}};
```

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

```
ListPlot[omn2]
```

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

```
Export["omn2", omn2, "Table"];
```

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

* Standard free energy change of reaction 3 (G3)

$$G3 = (dg_{sio2} + dg_{co} - dg_{sic} - dg_{O3});$$

* Equilibrium oxygen activity for reaction 3 (a3)

```
a3 = (G3 / (R * temp * 2.303)) + cod;
```

* Temperature - Equilibrium oxygen activity list for reaction 3 (eqbs3)

```
ozlw03 = {{temp[[1]], a3[[1]]}, {temp[[2]], a3[[2]]},
   {temp[[3]], a3[[3]]}, {temp[[4]], a3[[4]]}, {temp[[5]], a3[[5]]},
   {temp[[6]], a3[[6]]}, {temp[[7]], a3[[7]]}, {temp[[8]], a3[[8]]},
   {temp[[9]], a3[[9]]}, {temp[[10]], a3[[10]]}, {temp[[11]], a3[[11]]},
   {temp[[12]], a3[[12]]}, {temp[[13]], a3[[13]]}, {temp[[14]], a3[[14]]},
   {temp[[15]], a3[[15]]}, {temp[[16]], a3[[16]]}, {temp[[17]], a3[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 3*

```
ListPlot[ozlw03]
```

* Export data*

```
Export["ozlw03", ozlw03, "Table"];
```

* List of Temperature-Standard free energy change of reaction 3

```
omn3 = {{temp[[1]], G3[[1]]}, {temp[[2]], G3[[2]]},
   {temp[[3]], G3[[3]]}, {temp[[4]], G3[[4]]}, {temp[[5]], G3[[5]]},
   {temp[[6]], G3[[6]]}, {temp[[7]], G3[[7]]}, {temp[[8]], G3[[8]]},
   {temp[[9]], G3[[9]]}, {temp[[10]], G3[[10]]}, {temp[[11]], G3[[11]]},
   {temp[[12]], G3[[12]]}, {temp[[13]], G3[[13]]}, {temp[[14]], G3[[14]]},
   {temp[[15]], G3[[15]]}, {temp[[16]], G3[[16]]}, {temp[[17]], G3[[17]]}};
```

* Plot of Temperature-Standard free energy change of reaction 3*

```
ListPlot[omn3]
```

* Export list of Temperature-Standard free energy change of reaction 3*

```
Export["omn3", omn3, "Table"];
```

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4

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

■ * Standard free energy change of reaction 4 (G4)

$G4 = (dg_{sio2} + dg_{cgr} - dg_{sic} - 2/3 * dg_{O3});$

■ * Equilibrium oxygen activity for reaction 4 (a4)

```
a4 = (3 * G4) / (2 * R * temp * 2.303);
```

■ * Temperature - Equilibrium oxygen activity list for reaction 4 (eqbs4)

```
ozlw04 = {{temp[[1]], a4[[1]]}, {temp[[2]], a4[[2]]},
   {temp[[3]], a4[[3]]}, {temp[[4]], a4[[4]]}, {temp[[5]], a4[[5]]},
   {temp[[6]], a4[[6]]}, {temp[[7]], a4[[7]]}, {temp[[8]], a4[[8]]},
   {temp[[9]], a4[[9]]}, {temp[[10]], a4[[10]]}, {temp[[11]], a4[[11]]},
   {temp[[12]], a4[[12]]}, {temp[[13]], a4[[13]]}, {temp[[14]], a4[[14]]},
   {temp[[15]], a4[[15]]}, {temp[[16]], a4[[16]]}, {temp[[17]], a4[[17]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 4*

```
ListPlot[ozlw04]
```

■ * Export data*

```
Export["ozlw04", ozlw04, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 4

```
omn4 = {{temp[[1]], G4[[1]]}, {temp[[2]], G4[[2]]},
   {temp[[3]], G4[[3]]}, {temp[[4]], G4[[4]]}, {temp[[5]], G4[[5]]},
   {temp[[6]], G4[[6]]}, {temp[[7]], G4[[7]]}, {temp[[8]], G4[[8]]},
   {temp[[9]], G4[[9]]}, {temp[[10]], G4[[10]]}, {temp[[11]], G4[[11]]},
   {temp[[12]], G4[[12]]}, {temp[[13]], G4[[13]]}, {temp[[14]], G4[[14]]},
   {temp[[15]], G4[[15]]}, {temp[[16]], G4[[16]]}, {temp[[17]], G4[[17]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 4*

```
ListPlot[omn4]
```

■ * Export list of Temperature-Standard free energy change of reaction 4*

```
Export["omn4", omn4, "Table"];
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(* $\overset{5}{\text{SiC+ }} O_3$------> SiO + CO_2 *);

■ * Standard free energy change of reaction 5 (G5)

$G5 = (dg_{sio} + dg_{co2} - dg_{sic} - dg_{O3});$

■ * Equilibrium oxygen activity for reaction 5 (a5)

```
a5 = ((G5) / (R * temp * 2.303)) + co2d + siod;
```

■ * Temperature - Equilibrium oxygen activity list for reaction 5 (eqbs5)

```
ozlw05 = {{temp[[1]], a5[[1]]}, {temp[[2]], a5[[2]]},
   {temp[[3]], a5[[3]]}, {temp[[4]], a5[[4]]}, {temp[[5]], a5[[5]]},
   {temp[[6]], a5[[6]]}, {temp[[7]], a5[[7]]}, {temp[[8]], a5[[8]]},
   {temp[[9]], a5[[9]]}, {temp[[10]], a5[[10]]}, {temp[[11]], a5[[11]]},
   {temp[[12]], a5[[12]]}, {temp[[13]], a5[[13]]}, {temp[[14]], a5[[14]]},
   {temp[[15]], a5[[15]]}, {temp[[16]], a5[[16]]}, {temp[[17]], a5[[17]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 5*

```
ListPlot[ozlw05]
```

■ * Export data*

```
Export["ozlw05", ozlw05, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 5

```
omn5 = {{temp[[1]], G5[[1]]}, {temp[[2]], G5[[2]]},
   {temp[[3]], G5[[3]]}, {temp[[4]], G5[[4]]}, {temp[[5]], G5[[5]]},
   {temp[[6]], G5[[6]]}, {temp[[7]], G5[[7]]}, {temp[[8]], G5[[8]]},
   {temp[[9]], G5[[9]]}, {temp[[10]], G5[[10]]}, {temp[[11]], G5[[11]]},
   {temp[[12]], G5[[12]]}, {temp[[13]], G5[[13]]}, {temp[[14]], G5[[14]]},
   {temp[[15]], G5[[15]]}, {temp[[16]], G5[[16]]}, {temp[[17]], G5[[17]]}};
```

* Plot of Temperature-Standard free energy change of reaction 5*

```
ListPlot[omn5]
```

* Export list of Temperature-Standard free energy change of reaction 5*

```
Export["omn5", omn5, "Table"];
```

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```

$$\text{(*} \quad SiC^{6} + 1/3\, O_3\text{------>}\ SiO + C \quad \text{*);}$$

* Standard free energy change of reaction 6 (G6)

$$G6 = (dg_{sio} + dg_{cgr} - dg_{sic} - 1/3 * dg_{O3});$$

* Equilibrium oxygen activity for reaction 6 (a6)

```
a6 = (3 * G6) / (R * temp * 2.303) + 3 * siod;
```

* Temperature - Equilibrium oxygen activity list for reaction 6 (eqbs6)

```
ozlw06 = {{temp[[1]], a6[[1]]}, {temp[[2]], a6[[2]]},
   {temp[[3]], a6[[3]]}, {temp[[4]], a6[[4]]}, {temp[[5]], a6[[5]]},
   {temp[[6]], a6[[6]]}, {temp[[7]], a6[[7]]}, {temp[[8]], a6[[8]]},
   {temp[[9]], a6[[9]]}, {temp[[10]], a6[[10]]}, {temp[[11]], a6[[11]]},
   {temp[[12]], a6[[12]]}, {temp[[13]], a6[[13]]}, {temp[[14]], a6[[14]]},
   {temp[[15]], a6[[15]]}, {temp[[16]], a6[[16]]}, {temp[[17]], a6[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 6*

```
ListPlot[ozlw06]
```

* Export data*

```
Export["ozlw06", ozlw06, "Table"]
```

* List of Temperature-Standard free energy change of reaction 6

```
omn6 = {{temp[[1]], G6[[1]]}, {temp[[2]], G6[[2]]},
   {temp[[3]], G6[[3]]}, {temp[[4]], G6[[4]]}, {temp[[5]], G6[[5]]},
   {temp[[6]], G6[[6]]}, {temp[[7]], G6[[7]]}, {temp[[8]], G6[[8]]},
   {temp[[9]], G6[[9]]}, {temp[[10]], G6[[10]]}, {temp[[11]], G6[[11]]},
   {temp[[12]], G6[[12]]}, {temp[[13]], G6[[13]]}, {temp[[14]], G6[[14]]},
   {temp[[15]], G6[[15]]}, {temp[[16]], G6[[16]]}, {temp[[17]], G6[[17]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 6*

```
ListPlot[omn6]
```

■ * Export list of Temperature-Standard free energy change of reaction 6*

```
Export["omn6", omn6, "Table"];
```

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```

7

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

■ * Standard free energy change of reaction 7 (G7)

$$G7 = (dg_{si} + dg_{co2} - dg_{sic} - 2 / 3 * dg_{o3});$$

■ * Equilibrium oxygen activity for reaction 7 (a7)

```
a7 = ((3*G7) / (2*R*temp*2.303)) + (co2d);
```

■ * Temperature - Equilibrium oxygen activity list for reaction 7 (eqbs7)

```
ozlw07 = {{temp[[1]], a7[[1]]}, {temp[[2]], a7[[2]]},
   {temp[[3]], a7[[3]]}, {temp[[4]], a7[[4]]}, {temp[[5]], a7[[5]]},
   {temp[[6]], a7[[6]]}, {temp[[7]], a7[[7]]}, {temp[[8]], a7[[8]]},
   {temp[[9]], a7[[9]]}, {temp[[10]], a7[[10]]}, {temp[[11]], a7[[11]]},
   {temp[[12]], a7[[12]]}, {temp[[13]], a7[[13]]}, {temp[[14]], a7[[14]]},
   {temp[[15]], a7[[15]]}, {temp[[16]], a7[[16]]}, {temp[[17]], a7[[17]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 7*

```
ListPlot[ozlw07]
```

■ * Export data*

```
Export["ozlw07", ozlw07, "Table"];
```

* List of Temperature-Standard free energy change of reaction 7

```
omn7 = {{temp[[1]], G7[[1]]}, {temp[[2]], G7[[2]]},
   {temp[[3]], G7[[3]]}, {temp[[4]], G7[[4]]}, {temp[[5]], G7[[5]]},
   {temp[[6]], G7[[6]]}, {temp[[7]], G7[[7]]}, {temp[[8]], G7[[8]]},
   {temp[[9]], G7[[9]]}, {temp[[10]], G7[[10]]}, {temp[[11]], G7[[11]]},
   {temp[[12]], G7[[12]]}, {temp[[13]], G7[[13]]}, {temp[[14]], G7[[14]]},
   {temp[[15]], G7[[15]]}, {temp[[16]], G7[[16]]}, {temp[[17]], G7[[17]]}};
```

* Plot of Temperature-Standard free energy change of reaction 7*

```
ListPlot[omn7]
```

* Export list of Temperature-Standard free energy change of reaction 7*

```
Export["omn7", omn7, "Table"];
```

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8

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

* Standard free energy change of reaction 8 (G8)

$$G8 = (dg_{Si} + dg_{CO} - dg_{SiC} - 1/3 * dg_{O3});$$

* Equilibrium oxygen activity for reaction 8 (a8)

```
a8 = (3 * G8) / (R * temp * 2.303) + (cod * 3);
```

* Temperature - Equilibrium oxygen activity list for reaction 8 (eqbs8)

```
ozlw08 = {{temp[[1]], a8[[1]]}, {temp[[2]], a8[[2]]},
   {temp[[3]], a8[[3]]}, {temp[[4]], a8[[4]]}, {temp[[5]], a8[[5]]},
   {temp[[6]], a8[[6]]}, {temp[[7]], a8[[7]]}, {temp[[8]], a8[[8]]},
   {temp[[9]], a8[[9]]}, {temp[[10]], a8[[10]]}, {temp[[11]], a8[[11]]},
   {temp[[12]], a8[[12]]}, {temp[[13]], a8[[13]]}, {temp[[14]], a8[[14]]},
   {temp[[15]], a8[[15]]}, {temp[[16]], a8[[16]]}, {temp[[17]], a8[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 8*

```
ListPlot[ozlw08]
```

■ *** Export data***

```
Export["ozlw08", ozlw08, "Table"];
```

■ *** List of Temperature-Standard free energy change of reaction 8**

```
omn8 = {{temp[[1]], G8[[1]]}, {temp[[2]], G8[[2]]},
   {temp[[3]], G8[[3]]}, {temp[[4]], G8[[4]]}, {temp[[5]], G8[[5]]},
   {temp[[6]], G8[[6]]}, {temp[[7]], G8[[7]]}, {temp[[8]], G8[[8]]},
   {temp[[9]], G8[[9]]}, {temp[[10]], G8[[10]]}, {temp[[11]], G8[[11]]},
   {temp[[12]], G8[[12]]}, {temp[[13]], G8[[13]]}, {temp[[14]], G8[[14]]},
   {temp[[15]], G8[[15]]}, {temp[[16]], G8[[16]]}, {temp[[17]], G8[[17]]}};
```

■ *** Plot of Temperature-Standard free energy change of reaction 8***

```
ListPlot[omn8]
```

■ *** Export list of Temperature-Standard free energy change of reaction 8***

```
Export["omn8", omn8, "Table"];
```

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```

* Oxidation of Si*

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10 (* Si+1/3 O_3------> SiO *);

■ *** Standard free energy change of reaction 10 (G10)**

$$G10 = (dg_{sio} - dg_{si} - 1 / 3 * dg_{O3});$$

■ *** Equilibrium oxygen activity for reaction 10 (a10)**

```
a10 = (3 * G10) / (R * temp * 2.303) + 3 siod;
```

■ * Temperature - Equilibrium oxygen activity list for reaction 10 (eqbs10)

```
ozlw010 = {{temp[[1]], a10[[1]]}, {temp[[2]], a10[[2]]},
   {temp[[3]], a10[[3]]}, {temp[[4]], a10[[4]]}, {temp[[5]], a10[[5]]},
   {temp[[6]], a10[[6]]}, {temp[[7]], a10[[7]]}, {temp[[8]], a10[[8]]},
   {temp[[9]], a10[[9]]}, {temp[[10]], a10[[10]]}, {temp[[11]], a10[[11]]},
   {temp[[12]], a10[[12]]}, {temp[[13]], a10[[13]]}, {temp[[14]], a10[[14]]},
   {temp[[15]], a10[[15]]}, {temp[[16]], a10[[16]]}, {temp[[17]], a10[[17]]}};
```

■ * Plot of Temperature - Equilibrium oxygen activity list for reaction 10*

```
ListPlot[ozlw010]
```

■ * Export data*

```
Export["ozlw010", ozlw010, "Table"];
```

■ * List of Temperature-Standard free energy change of reaction 10*

```
omn10 = {{temp[[1]], G10[[1]]}, {temp[[2]], G10[[2]]},
   {temp[[3]], G10[[3]]}, {temp[[4]], G10[[4]]}, {temp[[5]], G10[[5]]},
   {temp[[6]], G10[[6]]}, {temp[[7]], G10[[7]]}, {temp[[8]], G10[[8]]},
   {temp[[9]], G10[[9]]}, {temp[[10]], G10[[10]]}, {temp[[11]], G10[[11]]},
   {temp[[12]], G10[[12]]}, {temp[[13]], G10[[13]]}, {temp[[14]], G10[[14]]},
   {temp[[15]], G10[[15]]}, {temp[[16]], G10[[16]]}, {temp[[17]], G10[[17]]}};
```

■ * Plot of Temperature-Standard free energy change of reaction 10*

```
ListPlot[omn10]
```

■ * Export list of Temperature-Standard free energy change of reaction 10*

```
Export["omn10", omn10, "Table"];
```

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11

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

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

G11 = (dg_{sio2} - dg_{si} - 2 / 3 * dg_{o3});

* Equilibrium oxygen activity for reaction 11 (a11)

```
a11 = (3 * G11) / (2 * R * temp * 2.303);
```

* Temperature - Equilibrium oxygen activity list for reaction 11 (eqbs11)

```
ozlw011 = {{temp[[1]], a11[[1]]}, {temp[[2]], a11[[2]]},
   {temp[[3]], a11[[3]]}, {temp[[4]], a11[[4]]}, {temp[[5]], a11[[5]]},
   {temp[[6]], a11[[6]]}, {temp[[7]], a11[[7]]}, {temp[[8]], a11[[8]]},
   {temp[[9]], a11[[9]]}, {temp[[10]], a11[[10]]}, {temp[[11]], a11[[11]]},
   {temp[[12]], a11[[12]]}, {temp[[13]], a11[[13]]}, {temp[[14]], a11[[14]]},
   {temp[[15]], a11[[15]]}, {temp[[16]], a11[[16]]}, {temp[[17]], a11[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 11*

```
ListPlot[ozlw011]
```

* Export data*

```
Export["ozlw011", ozlw011, "Table"];
```

* List of Temperature-Standard free energy change of reaction 11

```
omn11 = {{temp[[1]], G11[[1]]}, {temp[[2]], G11[[2]]},
   {temp[[3]], G11[[3]]}, {temp[[4]], G11[[4]]}, {temp[[5]], G11[[5]]},
   {temp[[6]], G11[[6]]}, {temp[[7]], G11[[7]]}, {temp[[8]], G11[[8]]},
   {temp[[9]], G11[[9]]}, {temp[[10]], G11[[10]]}, {temp[[11]], G11[[11]]},
   {temp[[12]], G11[[12]]}, {temp[[13]], G11[[13]]}, {temp[[14]], G11[[14]]},
   {temp[[15]], G11[[15]]}, {temp[[16]], G11[[16]]}, {temp[[17]], G11[[17]]}};
```

* Plot of Temperature-Standard free energy change of reaction 11*

```
ListPlot[omn11]
```

* Export list of Temperature-Standard free energy change of reaction 11*

```
Export["omn11", omn11, "Table"];

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```

* SiC equilibria*

****

```
(*    Si+ 14C ------> SiC   *);
```

- * Standard free energy change of reaction 14 (G14)

```
G14 = dgsic ;
```

- * List of Temperature-Standard free energy change of reaction 14

```
sds14 = {{temp[[1]], G14[[1]]}, {temp[[2]], G14[[2]]},
   {temp[[3]], G14[[3]]}, {temp[[4]], G14[[4]]}, {temp[[5]], G14[[5]]},
   {temp[[6]], G14[[6]]}, {temp[[7]], G14[[7]]}, {temp[[8]], G14[[8]]},
   {temp[[9]], G14[[9]]}, {temp[[10]], G14[[10]]}, {temp[[11]], G14[[11]]},
   {temp[[12]], G14[[12]]}, {temp[[13]], G14[[13]]}, {temp[[14]], G14[[14]]},
   {temp[[15]], G14[[15]]}, {temp[[16]], G14[[16]]}, {temp[[17]], G14[[17]]}};
```

- * Plot of Temperature-Standard free energy change of reaction 14*

```
ListPlot[sds14]
```

- * Export list of Temperature-Standard free energy change of reaction 14*

```
Export["sds14", sds14, "Table"];
```

```
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```

* Oxidation of C*

****

```
15 (*    C + 1/3 O3 ------>   CO            *);
```

- * Standard free energy change of reaction 15 (G15)

```
G15 = dgco - 1 / 3 * dgO3;
```

* Equilibrium oxygen activity for reaction 15 (a15)

```
a15 = (3 * G15) / (R * temp * 2.303) + (cod * 3);
```

* Temperature - Equilibrium oxygen activity list for reaction15 (eqbs15)

```
ozlw015 = {{temp[[1]], a15[[1]]}, {temp[[2]], a15[[2]]},
   {temp[[3]], a15[[3]]}, {temp[[4]], a15[[4]]}, {temp[[5]], a15[[5]]},
   {temp[[6]], a15[[6]]}, {temp[[7]], a15[[7]]}, {temp[[8]], a15[[8]]},
   {temp[[9]], a15[[9]]}, {temp[[10]], a15[[10]]}, {temp[[11]], a15[[11]]},
   {temp[[12]], a15[[12]]}, {temp[[13]], a15[[13]]}, {temp[[14]], a15[[14]]},
   {temp[[15]], a15[[15]]}, {temp[[16]], a15[[16]]}, {temp[[17]], a15[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 15*

```
ListPlot[ozlw015]
```

* Export data*

```
Export["ozlw015", ozlw015, "Table"];
```

* List of Temperature-Standard free energy change of reaction 15

```
omn15 = {{temp[[1]], G15[[1]]}, {temp[[2]], G15[[2]]},
   {temp[[3]], G15[[3]]}, {temp[[4]], G15[[4]]}, {temp[[5]], G15[[5]]},
   {temp[[6]], G15[[6]]}, {temp[[7]], G15[[7]]}, {temp[[8]], G15[[8]]},
   {temp[[9]], G15[[9]]}, {temp[[10]], G15[[10]]}, {temp[[11]], G15[[11]]},
   {temp[[12]], G15[[12]]}, {temp[[13]], G15[[13]]}, {temp[[14]], G15[[14]]},
   {temp[[15]], G15[[15]]}, {temp[[16]], G15[[16]]}, {temp[[17]], G15[[17]]}};
```

* List of Temperature-Standard free energy change of reaction 15

```
ListPlot[omn15]
```

* Export list of Temperature-Standard free energy change of reaction 15*

```
Export["omn15", omn15, "Table"];
```

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```

```
                16
(*    C + 2/3*O3 ------>   CO2     *);
```

* Standard free energy change of reaction 16 (G16)

```
G16 = G16CO2 = dgco2 - 2 / 3 * dgO3   ;
```

* Equilibrium oxygen activity for reaction 16 (a16)

```
a16 = (3 * G16 / (2 * R * temp * 2.303)) + 3 / 2 * co2d;
```

* Temperature - Equilibrium oxygen activity list for reaction 16 (eqbs16)

```
ozlw016 = {{temp[[1]], a16[[1]]}, {temp[[2]], a16[[2]]},
   {temp[[3]], a16[[3]]}, {temp[[4]], a16[[4]]}, {temp[[5]], a16[[5]]},
   {temp[[6]], a16[[6]]}, {temp[[7]], a16[[7]]}, {temp[[8]], a16[[8]]},
   {temp[[9]], a16[[9]]}, {temp[[10]], a16[[10]]}, {temp[[11]], a16[[11]]},
   {temp[[12]], a16[[12]]}, {temp[[13]], a16[[13]]}, {temp[[14]], a16[[14]]},
   {temp[[15]], a16[[15]]}, {temp[[16]], a16[[16]]}, {temp[[17]], a16[[17]]}};
```

* Plot of Temperature - Equilibrium oxygen activity list for reaction 16*

```
ListPlot[ozlw016]
```

* Export data*

```
Export["ozlw016", ozlw016, "Table"];
```

* List of Temperature-Standard free energy change of reaction 16

```
omn16 = {{temp[[1]], G16[[1]]}, {temp[[2]], G16[[2]]},
   {temp[[3]], G16[[3]]}, {temp[[4]], G16[[4]]}, {temp[[5]], G16[[5]]},
   {temp[[6]], G16[[6]]}, {temp[[7]], G16[[7]]}, {temp[[8]], G16[[8]]},
   {temp[[9]], G16[[9]]}, {temp[[10]], G16[[10]]}, {temp[[11]], G16[[11]]},
   {temp[[12]], G16[[12]]}, {temp[[13]], G16[[13]]}, {temp[[14]], G16[[14]]},
   {temp[[15]], G16[[15]]}, {temp[[16]], G16[[16]]}, {temp[[17]], G16[[17]]}};
```

* List of Temperature-Standard free energy change of reaction 16

```
ListPlot[omn16]
```

* Export list of Temperature-Standard free energy change of reaction 16*

```
Export["omn16", omn16, "Table"];

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 xxxxxxxxxxxxxxxx
```