

Verification of the Possibility of Producing Wüstite From the Decomposition of Hematite and Magnetite in the Inner Layers of the Earth

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Abstract:

This research aims, starting from the study of the change in the free energy of a chemical reaction, to reveal the possibility of producing one of the important oxides in the formation of the Earth's layers, especially the Earth's lower mantle. This oxide is FeO or what is name Wüstite, which can be produced from the decomposition of each of Hematite (Fe_2O_3), Magnetite (Fe_3O_4). This is done by calculating and taking into account three important hypotheses, which are the change and stability with the change in temperature from 0 to 7000 °C for each of the thermodynamic parameters, which are; heat capacity at constant pressure, enthalpy and entropy of reaction. What we found from it; that our study indicates that the production of this oxide through the decomposition of hematite occurs at all depths of the Earth, starting from the Earth's crust. While its production from the decomposition of magnetite continues regardless of the depth of the Earth, but this is mostly from specific depths. As long as the three parameters do not change with the change in temperature, this production begins approximately from the middle of the Earth's lower mantle and precisely from the depth 1497.3 km, but as long as the heat capacity does not change with constant pressure, production begins from the middle of the Earth's crust, and precisely from the depth 27.93 km. Finally, and with the change of all parameters together with the change in temperature, this begins from the depth 77.89 km which corresponds to the beginning of the lithosphere region.

Keywords: Wüstite, Hematite, Magnetite, chemical reaction, free energy, geophysics

I- Introduction:

Chemical reactions can decide to produce substances and destroy others, including decomposition, oxidation, nitration and hydrogenation reactions... etc. This is according to the thermodynamic conditions, especially pressure and temperature. The temperature at which the spontaneous reaction begins to produce one substance

from another or several substances is sought. This is done by observing the evolution of the Gibbs free energy of the reaction with the change in temperature, the latter increasing as we go deeper into the Earth, as will be shown later.

In another way, knowledge of the deep structure of the Earth has been revealed - mainly indirectly - thanks to the contribution of several disciplines of the Earth sciences, which cannot deal, in detail, with the contribution of each of these disciplines we will limit ourselves here to briefly mention the principle of these methods giving their main results [01].

1- Seismological Model of the Earth or seismology, it is the study of natural and artificial earthquakes. From the results of these works, in the two categories of subdivisions used in parallel for the interior of the globe can be distinguished. This is well covered by the work of Dziewonski AM, Anderson DL (1982) [02], which are summarized in the PREM (Preliminary reference Earth model).

a)- Based on the major discontinuities of seismic wave speeds; Based on the major discontinuities highlighted by the abrupt variation in the speed of seismic waves of the Earth's globe allows us to distinguish from the outside to the inside; The crust is the outer layer that represents 1.5% of the Earth's volume. It is limited at the base by the major discontinuity of Mohorovicic (called Moho). It is necessary to distinguish 2 types of crust; the continental crust, 35 km thick on average (but can reach 70 km under high mountain ranges). The oceanic crust, very thin (5 to 8 km under the oceans). The differences in thickness of the crust are closely linked to isostasy phenomena, which involve differences in the density of rocks. The mantle: it represents 82.5% of the Earth's volume. It is 2900 km thick. It is limited at the base by the major Gutenberg discontinuity. Within this mantle, we can distinguish 2 units; the upper mantle which extends up to 670 km. The lower mantle whose depth is between 670 km and 2900 km. The Core; it represents 16% of the Earth's globe. The core has a maximum thickness of 3300 km. It includes; the outer core, whose depth is between 2900 km and 5150 km. The inner core (or Seed), whose depth is between 5150 km and 6370 km [03].

b)- Based on the physical behavior of the layers When we take into account the physical behavior of materials, depending on whether they behave like rigid materials or like "soft" materials, we distinguish: The lithosphere which is a rigid block and which includes the crust and the rigid upper part of the upper mantle. Its thickness varies between 5 km under the oceans and 100 km at the level of the continents. Its lower limit is marked by a discontinuity of the seismic waves called LVZ (Low Velocity Zone). The asthenosphere, which is a "soft" or "plastic" zone which extends from the lower limit of the lithosphere to a depth of 670 km. It is formed from the rest of the upper mantle, the upper part of which is a zone of lower seismic wave speed (LVZ) whose thickness is approximately 200 km. The mesosphere is a "rigid" block; it is synonymous with the lower mantle. Its upper limit (670 km) is marked by the sudden increase in seismic wave speeds up to the Gutenberg discontinuity (2900 km), its density also increases with this depth. The D'' layer was highlighted thanks to the detailed study of longitudinal P wave transmissions during a strong earthquake. It is a soft zone, 200 to 300 km thick, between the lower mantle and the outer core. Its role is currently enigmatic. The outer core is a liquid layer between the D'' layer and the Lehman discontinuity, its density increases with depth. The inner core is a solid layer called seed [04].

2- Thermal Model of the Earth; The temperature increases with depth. We speak of a geothermal gradient, which is equal on average to 10°C/km in the stable zones of the continental crust and to 30°C/km in the deformation zones. If the gradient were constant in depth we would end up with a very very high temperature, incompatible with its solid state of the seed. The production of internal heat by the Earth is essentially the consequence of radioactive disintegration. The average flow of internal heat is approximately 70 MW/m², or a total of 42.3TW (1TW = 1000 GW). The heat flow is the quantity of heat, in Joule, crossing the unit of surface per unit of time (J./s/m² = W./m²). The transport of heat from the inside to the outside is a complex process that occurs mainly by conduction in the thermal boundary layers (lithosphere, core-mantle boundary) and by convection on the geological time scale in the layers capable of deforming by creep (mantle, core). The internal energy produced by the Earth is the source of all internal phenomena that occur there; plate tectonics, earthquakes, volcanism, variation of the Earth's magnetic range and the gravity range. The temperature profile as a function of depth (called geothermal) [05].

3- Geochemical, Mineralogical Model of the Earth. The chemical and mineralogical composition of materials inside the Earth is well known for the first 250 km of depth of the Earth thanks to the direct study; peridotites which are rocks formerly deep, but now visible on the surface following their uplift (by the obduction mechanism) and the erosion of the terrains which hid them; basalts and its peridotite enclaves whose magma is located in the mantle at different depths. Beyond 250 km the chemical and mineralogical composition is currently known indirectly by the study. Materials by compressing for example the peridotites between two

diamond cells with pressures and temperatures equivalent to those of the different zones of the mantle. Transmission speeds of seismic waves in different materials by comparing the results with the speeds obtained during an earthquake. The studies of differentiated meteorites as well as experimental seismology have provided an idea of the chemical composition of the nucleus [06].

The main constituents of the crust are silica SiO_2 (50 to 60% on average) and Alumina (Al_2O_3) (15 to 16% on average). For this reason, the crust is referred to as SIAL. Among the other constituents; which have been determined in the form of oxides, which are in much lower percentage; we can mainly cite CaO , MgO , FeO . These last three are more abundant in the oceanic crust and in the lower part of the continental crust than in the upper continental crust. Because the proportion of silica exceeds a certain percentage, the upper continental crust is called "acid". And it is mainly made up of Quartz + Feldspars + Pyroxenes. Because the proportion of silica is lower than a certain percentage of the lower continental crust and the oceanic crust, which are called "basic". Quartz + Pyroxenes + Oxides. The superficial part of the upper continental crust (a few thousand meters) is mainly made up of sediments and sedimentary rocks metamorphosed at the base of this part, but the bulk is formed of granitic magmatic rocks, hence sometimes the name "granitic" crust and metamorphic rocks [06].

The mantle has less silica (only 40% of its composition) than in the crust; it is therefore very "basic". It contains a high proportion of magnesium; hence the name SIMA for the mantle. Its upper part is made up of peridotites and its lower part probably has the same composition as the upper mantle but the atoms are assembled in denser (more compact) structures due to the increase in pressure. From a mineralogy point of view; the top of the upper mantle is made up of Olivine + Pyroxenes + Oxides. The base of the upper mantle is made up of Spinel (very dense Olivine) + Pyroxenes + Oxides. The lower mantle is made up of Perovskite (very very dense Olivine) + Oxides [07].

The inner core would be made up of siderophile elements; lots of iron, nickel, cobalt, gold, platinum, etc. The outer ("liquid") core would be made up of a high proportion of iron associated with light elements such as oxygen, sulfur; and a little silica [07].

Through this mineralogical model, the importance of iron oxide becomes clear, as a pure electrode on the one hand and as a component of the mineral MW that enters the formation of the lower mantle of the Earth. This oxide has been the subject of many studies, from a geophysical perspective, including; Brown, J. M., & Shankland, T. J. (1981) [09], Yagi, T et al (1988) [10], Fei, Y., & Mao, H. K. (1994) [11], Murakami, M et al (2004) [12], Kolorenč, J., & Mitás, L. (2008) [13], Ozawa, H et al (2010) [14], Fischer, R et al (2011) [15], Tlili, S et al 2017 [16] and Tanaka, R at al (2020) [17]. But despite the multiplicity of these studies dealing with this oxide, whether experimental or computational, they are reports that lack clarification of how this oxide is formed in the inner layers of the Earth.

In this computational study, we are interested in identifying the developments of enthalpy and entropy of reaction and thus its free energy with the change in temperature of the Earth's interior. This is in order to produce iron oxide from the elements hematite and magnetite, with three assumptions: first, the enthalpy, entropy of reaction and heat capacity are constant with the volume constant with the change in temperature, second, only the heat capacity is constant with the volume constant with the change in temperature, and finally, all of them change with the change in temperature. Therefore, we continue this introduction with a descriptive statement of the study method, followed by a presentation and discussion of the results and finally a conclusion.

II- Method study:

It is known that any reaction is a transformation of compounds from reactants (R_i) to products (P_i) according to the following equation [18]:



where; n_i number of moles of reactants and n_j number of moles of products.

Each reaction is accompanied by a change in the following state function.

The enthalpy function: The difference between the potential energy level of the products and the potential energy of the reactants is known as the heat of the chemical reaction, and is symbolized by the symbol (ΔH). Therefore, when the value of the heat of reaction is positive, the reaction is endothermic, while the negative value means that the reaction is exothermic. There are several types that are often subject to the type of reaction. Of these types, only the standard enthalpy of formation is enough, which is known as the change in enthalpy

when forming one mole of the compound from its initial elements. These elements are usually found in their standard state, and the heats of formation of the compounds used in a chemical reaction have an important relationship with the heat of reaction. For computational purposes, it has been agreed that the heat of formation is equal to zero for all elements in their standard states at all temperatures. The enthalpy of a compound is then equal to its heat of formation. On this basis, the heat change of any reaction can be calculated by knowing the heats of formation of the materials participating in this reaction and resulting from it. If the heats of formation of all chemical compounds were complete, the heat of any reaction could be calculated without performing it practically in a calorimeter. In the general form, the heat of reaction can be expressed as follows [19]:

$$\Delta H_{\text{Reaction}} = \sum_i n_i \Delta H_{\text{productants}_i} - \sum_j n_j \Delta H_{\text{Reactants}_j} \quad (2)$$

Entropy describes the degree of disorder and irregularity of particles, or ΔS is a thermodynamic property of the order of the system and the dispersion of energy associated with these particles. The less order in the system (greater randomness), the greater the value of entropy and the more orderly the system (less randomness), the smaller the value of entropy. Chemists use it to know whether a chemical reaction can occur spontaneously or not, under certain conditions of pressure and temperature. Where the standard entropy ΔS is the difference between the sum of the standard entropy values of all products and the sum of the standard entropy values of all reactants. It is calculated for reactions as in the previous expression as follows [19]:

$$\Delta S_{\text{Reaction}} = \sum_i n_i \Delta S_{\text{productants}_i} - \sum_j n_j \Delta S_{\text{Reactants}_j} \quad (3)$$

Finally, ΔG is the free enthalpy of Gibbs free energy, which is a thermodynamic property that combines the entropy and enthalpy of a system in order to determine whether a reaction is spontaneous. If it is positive, it means that the reaction is non-spontaneous and requires external intervention to occur and vice versa. If its value is negative, the reaction is spontaneous. Therefore, its change is calculated using the following relationship [20]:

$$\Delta G_{\text{reaction}} = \Delta H_{\text{reaction}} - T \cdot \Delta S_{\text{reaction}} \quad (4)$$

These three functions (ΔH , ΔS , ΔG) are related to the temperature of the reaction medium, as the relationship (4) shows the relationship of free energy to temperature. While both enthalpy and entropy change with temperature according to the following two Kirchhoff relationships [20]:

$$\Delta H_{\text{reaction}}(T) = \Delta H_{\text{reaction}}(298) + \int \Delta C_{p_{\text{reaction}}} dT \quad (5)$$

$$\Delta S_{\text{reaction}}(T) = \Delta S_{\text{reaction}}(298) + \int \Delta C_{p_{\text{reaction}}} \frac{dT}{T} \quad (6)$$

Also, the heat capacity changes with temperature for each substance according to the following general relationship [21]:

$$C_p = aT^3 + bT^2 + cT + d \quad (7)$$

where the values of the coefficients a , b , c and d are from the available data tables such as the handbook, however, they change for any reaction according to the following relationship [21]:

$$\Delta C_{p_{\text{Reaction}}} = \sum_i n_i C_{p_{\text{productants}_i}} \rightarrow \sum_j n_j C_{p_{\text{Reactants}_j}} \quad (8)$$

In this study, we will study the change of these functions in terms of temperature in the different internal layers of the Earth's interior, with the aim of knowing the depth at which the spontaneous reaction begins and the extent to which this spontaneity is maintained. Considering that the pressure is constant and the only variable is the temperature depending on the depths of the Earth, which changes from 298 to 7000 K. So here we are looking for when it is achieved; $\Delta G_{\text{reaction}} < 0$, in other words we are in the process of determining the value of T_c the temperature that achieves this, i.e. at what depth it occurs. And in order for this study to have more accurate and broad results, we will take the following probabilities for this reaction:

- 1- Change in temperature only without changing enthalpy, entropy and heat capacity.
- 2- Change in enthalpy, entropy with temperature change without changing heat capacity.

3- Change in enthalpy, entropy and heat capacity with temperature change.

All this is in order to study the possibility of producing iron oxide or Wüstite from Hematite and Magnetite, which is subject to the following two chemical equations [19-21]:

The first reaction or producing Wüstite from Hematite:



The second reaction or producing Wüstite from Magnetite:



For these four materials, we present in Table (1) the values of enthalpy, entropy and heat capacity at constant pressure at room temperature, in addition to the values of the coefficients of change of the latter with temperature changes.

This study method generally requires hard work, but two basic points can be adopted to facilitate the work, which are:

Using an analytical method to calculate the values of the previous integrals, including the midpoint Rule [22], trapezoidal Rule [23], Simpson Rule [24] and Romberg Rule [25]. Whose values are equal for a very large number of iterations, which the computer can handle with ease.

We can use any programming language such as FORTRAN or a development environment such as Silab or Matlab to create a simple program that enables us to calculate.

Table (1) shows the enthalpy values of the two studied reactions when the heat capacity is constant and changes in the most important boundaries of the deep earth layers.

	Fe2O3 (s)	Fe2O4 (s)	O2 (g)	FeO (s)
n(mole)	2	2	1	4
$\Delta h_f^\circ, 298(\text{kJ. mol}^{-1})$	-	-	0	-
$s^\circ 298(\text{J. K}^{-1} \cdot \text{mol}^{-1})$	8,99,775	1,46,475	16,74,12,555	59,427
$C_p^\circ 298(\text{J. K}^{-1} \cdot \text{mol}^{-1})$	4603,5	4603,5	6277,5	5022
a	9,77,616	1,67E+02	3,61,70,955	159,03
b	0,0721494	0,0789291	0,00084537	0,00678
c	0	0,00E+00	0	0
d	-1288980	-4189185	-426870	-308853

III- Results and discussion:

In all figures presented here the letters represent the following: A - the surface we live on, B - the end of the continental crust, C - the end of the lithosphere region, D - the boundary between the upper and lower mantle, E - the boundary between the Earth's lower mantle and the Earth's outer core, F - the boundary between outer and the Earth's inner core, G the center of the Earth's cavity.

III-1 The enthalpy changes of the Reaction:

Figure (1) shows the change in the heat content of the two studied reactions, when the heat capacity of the two studied reactions is constant and when the temperature changes in the depths of the Earth.

Figure (2) shows the change in the enthalpy of the two studied reactions, when the heat capacity changes when the temperature changes in the depths of the Earth.

Table (2) shows the enthalpy values of the studied reactions at constant and variable heat capacity at the main boundaries of the deep Earth's layers.

Figure (1) shows the change in the enthalpy of formation for the two reactions with the change in the temperature of the subsurface and thus the subsurface depth, with the heat capacity fixed with the change in temperature for a constant pressure. From this it is clear that both reactions absorb heat, especially after the estimated depth of 20.32 km for the first reaction the previous reaction is exothermic. Moreover, the amounts of

this enthalpy are limited between $-17.49 \cdot 10^{-2}$ Mjoule and 114.82 Mjoule for the first reaction, while they are limited between $-63.53 \cdot 10^{-2}$ Mjoule and 182.95 Mjoule for the second reaction. In addition, it is clear that both reactions absorb a very close amount of heat, as the value of the difference in this enthalpy at the surface of the earth's crust is estimated at $81.02 \cdot 10^{-2}$ Mjoule. It also appears from this figure and the values of Table (1) that with increasing penetration into the subsurface the value of the absorbed heat increases, linearly for both reactions, but this increase is slower for the first reaction with the lowest absorption as well compared to the absorption of the other reaction, where the absorption tendencies 24.46 Mjoule/K and 38.77 Mjoule/K are respectively estimated at and. This makes the difference between the absorption values also increasing, whose value reaches 68.13 Mjoule at the center of the earth's interior.

For the heat capacity at constant pressure and variable with temperature, the changes in the reaction heat are also represented for both reactions, as it turns out in Figure (2) and the Table (2). Through them, it can be noted that this heat is absorbed, but always starts from the depth 49.75 km for the first reaction. However the values of this heat and for both reactions maintain, the same previous position and the difference in its values between the two reactions are also increasing. Where the value of this difference at the surface of the Earth's crust is estimated at 810.22 kjoule, while it is estimated at 2.01 Mjoule in the center of the Earth's interior. Moreover, the heat of absorption changes over a wide range, the width of which is given at the value 831.43 kjoule for the first reaction, and at the value 1.66 Mjoule for the second reaction. But the shape of the change here takes the form of an inverted parabola, especially for the first reaction. Where its maximum value reaches the value 656.50 kjoule at the depth 2466.9 K, that is, on the borders of the Earth's outer core and after the end of the Earth's lower mantle, corresponding to a temperature estimated at 4098 K. As for the second reaction, the value 2.29 Mjoule of the absorbed heat is at their maximum value at the beginning of the Earth's inner core, that is, at the depth estimated at 5216.8 km and corresponding to a temperature estimated at 5638 K.

Finally, through these two figures and this table, it can be noted that if the heat capacity is constant with a change in temperature and the pressure is constant. The values of the absorbed heat are much higher than their values in the other case of the heat capacity.

Table (2) shows the heat content values for the two reactions studied when the heat capacity is constant and variable in the most important boundaries of the deep layers of the Earth.

Major Discontinuities	Depth (km)	Temperature (°C)	ΔH (kJ/mole)			
			Fe ₂ O ₃ (Mj/mole)		Fe ₃ O ₄ (kj/mole)	
			Cp=Cte	C=f(T)	Cp=Cte	C=f(T)
Surface we live	A 0	298	-17,49E-2	-174,93	63,53E-2	63,53E-2
Base of Continental Crust	B 70	1000	11,87	105,10	19,73	1051,53
Base of Lithosphere	C 100	1350	17,88	222,76	29,25	1232,36
Limit Upper and Lower Mantle	D 670	1600	22,17	298,12	36,05	1352,50
Limit Lower Mantle and Outer Core	E 2900	4700	75,36	635,70	120,38	2239,91
Limit Outer Core and inner core	F 5100	5500	89,08	543,69	142,14	2289,39
Center of the Earth's Cavity	G 6370	7000	114,82	173,14	182,95	2184,06

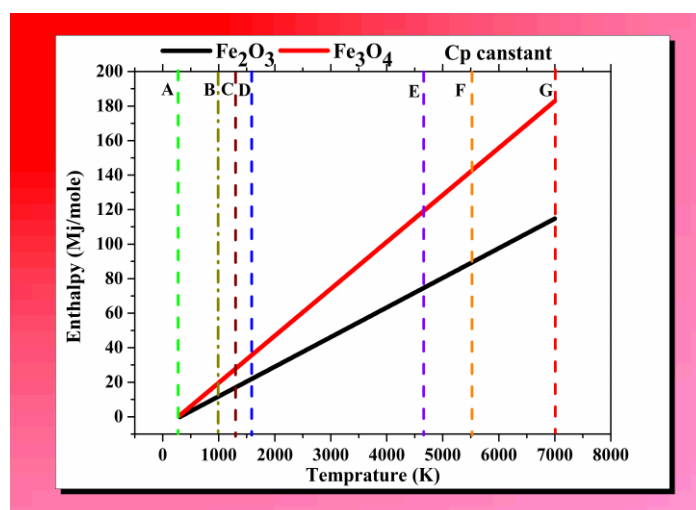


Figure (1) shows the change in the enthalpy of the two studied reactions, when the heat capacity of the two studied reactions is constant with the difference in temperatures in the Earth's depths.

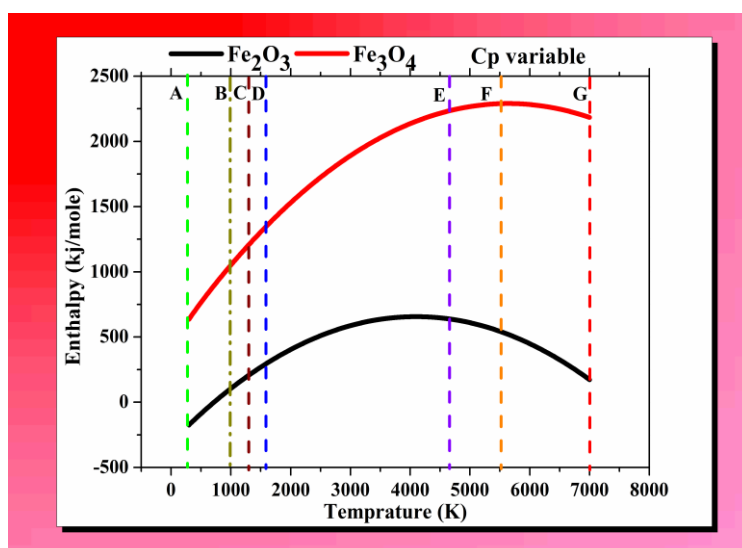


Figure (2) shows the change in the enthalpy of the two studied reactions with the change in heat capacity at varying temperatures in the Earth's depths.

III-2 The entropy changes of the reaction:

Figures (3 and 4) illustrate the change in the entropy of the reaction or randomness with a change in the depth of the Earth's interior or its temperature. The first represents the case in which the heat capacity is constant at constant pressure and does not change with a change in temperature, while the second represents the case in which this capacity changes with a change in temperature. Through them and the values recorded in Table (3), it is noted that there is Preservation in the positioning of the values of this randomness and an increase in the difference between its values for the two reactions, as was the case with the absorbed heat.

Figure (3) shows the change in entropy of the two studied reactions, when the heat capacity is constant when the temperature changes in the depths of the Earth.

Figure (4) shows the change in entropy of the two studied reactions when the heat capacity changes when the temperature changes in the depths of the Earth.

Table (3) Entropy values of the two studied reactions when is constant and changes the heat capacity in the most important boundaries of the earth's layers.

In addition, the increase in entropy in both reactions and in both cases of heat capacity at constant pressure is faster from the surface to the beginning of the lower mantle. After that, up to Earth's interior center of the interior, the increase continues but slowly in at first case, where this change is within two ranges whose values are 54.16 kJoule/K and 85.87 kJoule/K for the two reactions, respectively.

Table (3) shows the entropy values of the studied reactions at constant and varying heat capacity in the main boundaries of the deep Earth's layers.

Major Discontinuities	Depth (km)	Temperature (°C)	ΔS			
			Fe_2O_3		Fe_3O_4	
			$\text{Cp}=\text{Cte}$ (kJ/Kmole)	$\text{C}=\text{f}(\text{T})$ (j/Kmole)	$\text{Cp}=\text{Cte}$ (kJ/Kmole)	$\text{C}=\text{f}(\text{T})$ (j/Kmole)
Surface we live	A 0	298	22,52E-2	225,17	22,10E-2	231,02
Base of Continental Crust	B 70	1000	20,10	716,60	33,16	961,71
Base of Lithosphere	C 100	1350	26,15	815,66	41,33	1113,84
Limit Upper and Lower Mantle	D 670	1600	29,06	865,21	45,95	1192,92
Limit Lower Mantle and Outer Core	E 2900	4700	47,55	989,12	75,26	1494,48
Limit Outer Core and inner core	F 5100	5500	50,25	963,50	79,54	1492,85
Center of the Earth's Cavity	G 6370	7000	54,39	889,96	86,10	1454,65

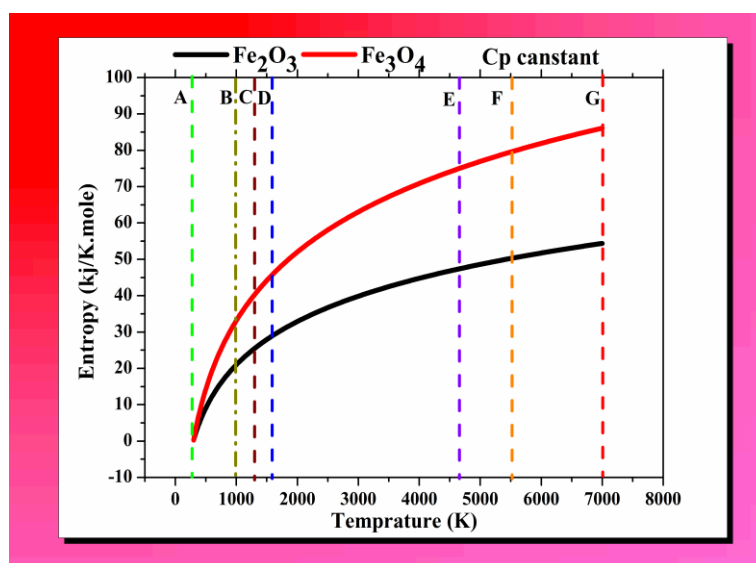


Figure (3) shows the change in the entropy of the two studied reactions, when the heat capacity is constant when the temperature changes in the Earth's depths.

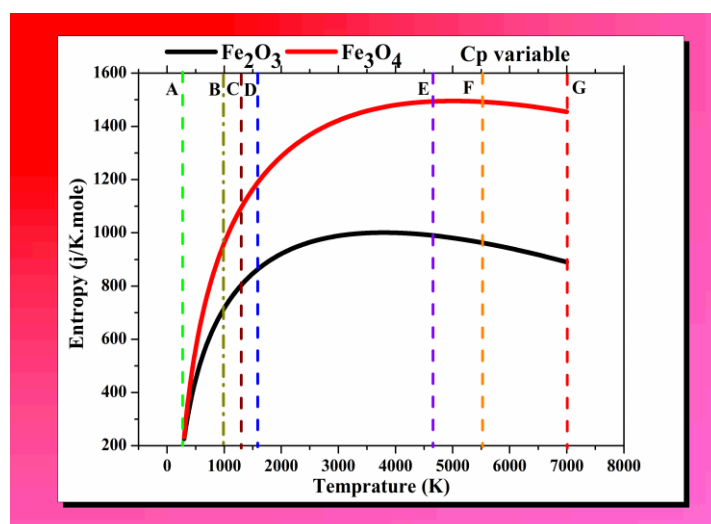


Figure (4) shows the change in the entropy of the two studied reactions, when the heat capacity changes when the temperature changes in the depths of the Earth.

For the second case of constant pressure heat capacity (see Figure (4)), the increase in randomness continues from the surface of the Earth's crust to the depth 2246.8 km which is located within the Earth's lower mantle, corresponding to the temperature estimated at 3792 K for the first reaction. At this depth, the value of randomness is estimated at 1 kJoule/K, but after this depth, randomness begins to decrease until the center of the Earth's interior, where the value of this randomness is estimated at 86.10 joule/K. For the second reaction, the increase in this randomness also continues to increase from the surface of the Earth's crust to the beginning of the Earth's outer core, where its value reaches its maximum estimated at 1.5 kJoule/K. And that is exactly at the depth estimated at 3752.5 km corresponding to the temperature whose value is 5010 K. For this case, the amount of randomness changes within two range whose values are respectively 775.76 joule/K and 1264.77 joule/K.

It can also be noted that the entropy value for the first case of heat capacity has higher values than that for the second case.

III-3 The Free energy changes of the reaction:

Table (4) Free energy values for the two reactions studied when the constant and changes heat capacity in the most important boundaries of the deep layers of the Earth.

Figure (5) shows the change in the Free energy of the two studied reactions, when the heat capacity is constant when the temperature changes in the depths of the Earth.

Figure (6) shows the change in the Free energy of the two studied reactions, when the heat capacity changes when the temperature changes in the depths of the Earth.

Figure (7) shows the change in the Free energy of the reaction when the heat capacity of the two reactions studied is constant when the temperature changes in the depths of the Earth.

Figures (5-7) show the change in the free energy or Gibbs energy of the two reactions with changes in the depth of the Earth's interior or the temperature of the Earth's interior. The first is when the enthalpy, entropy of the reaction and heat capacity do not change with constant pressure and temperature. The second is when the heat capacity does not change with constant pressure and change in temperature. Finally, they all change with temperature. From these figures, it is clear that the values of this energy for the second reaction are higher than their values for the first reaction, and it is a constantly decreasing energy

In the first case, as is clear from Figure (5), the decrease is almost linear for both reactions, as the speed rates of this decrease appear to be almost equal. Their values are estimated by 0.32 MJoule/K for the first reaction and by 0.33 MJoule/K for the second reaction. The difference between the values of this energy when comparing the two reactions is also almost equal, as it is estimated at the surface of the Earth's crust by 0.81 MJoule and it is estimated at 0.77 MJoule at the center of the Earth's interior. It also appears that for the first reaction, this

decomposition reaction is achieved regardless of the depth, i.e. it is achieved from the surface to the center. As for the second reaction, the decomposition reaction is spontaneous starting from the depth 1497.3 km corresponding to the temperature estimated by 2750 K, i.e. at a depth slightly close to the middle of the Earth's lower mantle, the decomposition reaction begins to occur. In addition, this energy is variable within the two ranges, whose values are - 1.5 MJoule and 1.55 MJoule for each reaction, respectively.

In the second case, starting from the value - 0.24 MJoule for the first reaction and the value 0.57 MJoule for the second reaction, i.e. the energy value is initially almost identical. However, the first reaction always is spontaneous, while up to the depth 27.93 km corresponding to the estimated temperature at 414 K. These two depths are within the range of the Earth's crust. Immediately after them, the difference between the energy values of each reaction begins to increase continuously due to the non-linear decrease in their values, where this difference is estimated at the center of the Earth's interior. Moreover, the amounts of this energy are limited within the two the ranges estimated by 265.65 MJoule and 420.13 MJoule for the two reactions, respectively.

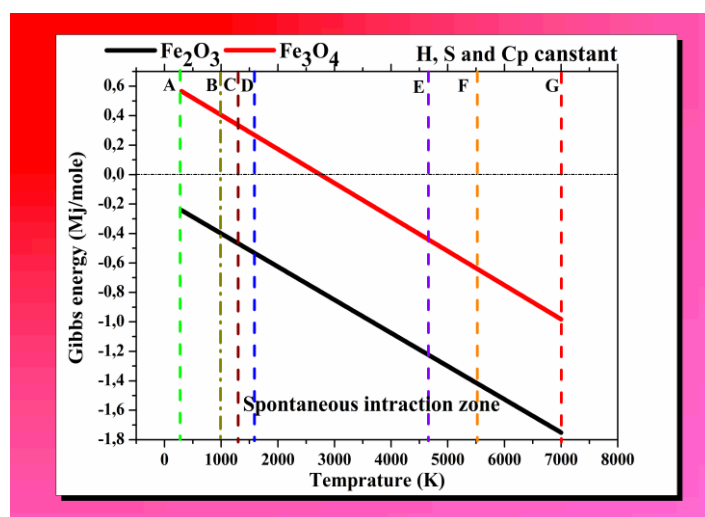


Figure (5) shows the change in entropy of the two studied reactions, when the heat capacity is constant when the temperature changes in the Earth's depths.

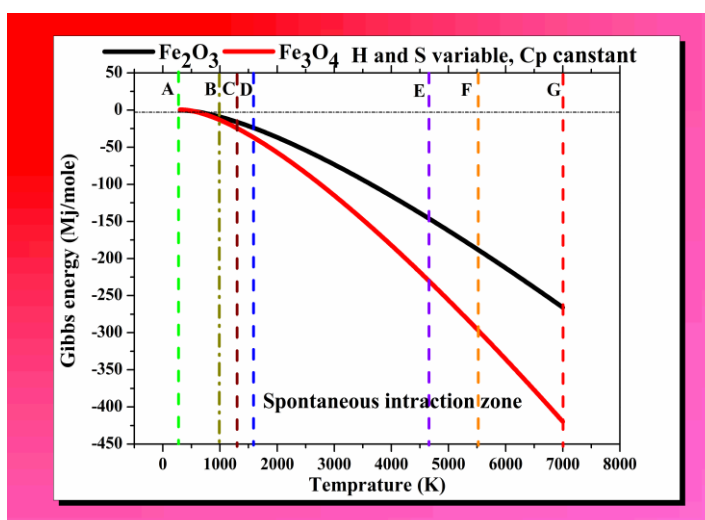


Figure (6) shows the entropy change of the two reactions studied, when the heat capacity changes when the temperature changes in the Earth's depths.

Table (4) shows the free energy values for the two studied reactions at constant and varying heat capacity at the main boundaries of the deep Earth's layers.

Major Discontinuities	Depth (km)	Temperature (°C)	$\Delta G(\text{Mj/mole})$						
			Fe_2O_3			Fe_3O_4			
			$\text{H}_2\text{S}=\text{f}(\text{T})$	$\text{C}_p=\text{f}(\text{T})$	$\text{H}_2\text{S}, \text{C}_p=\text{Cte}$	$\text{H}_2\text{S}=\text{f}(\text{T})$	$\text{C}=\text{f}(\text{T})$	$\text{H}_2\text{S}=\text{f}(\text{T})$	
Surface we live	A 0	298	-0,24	-0,24	0,57	0,57	0,57	-0,24	
Base of Continental Crust	B 70	1000	-9,13	-0,61	0,40	-13,43	0,09	-9,13	
Base of Lithosphere	C 100	1350	-17,42	-0,88	0,32	-26,54	-0,27	-17,42	
Limit Upper and Lower Mantle	D 670	1600	-24,34	-1,09	0,27	-37,47	-0,56	-24,34	
Limit Lower Mantle and Outer Core	E 2900	4700	-148,14	-4,01	-0,45	-233,35	-4,78	-148,14	
Limit Outer Core and inner core	F 5100	5500	-187,29	-4,76	-0,64	-295,31	-5,92	-187,29	
Center of the Earth's Cavity	G 6370	7000	-265,89	-6,06	-0,98	-419,74	-8,00	-265,89	

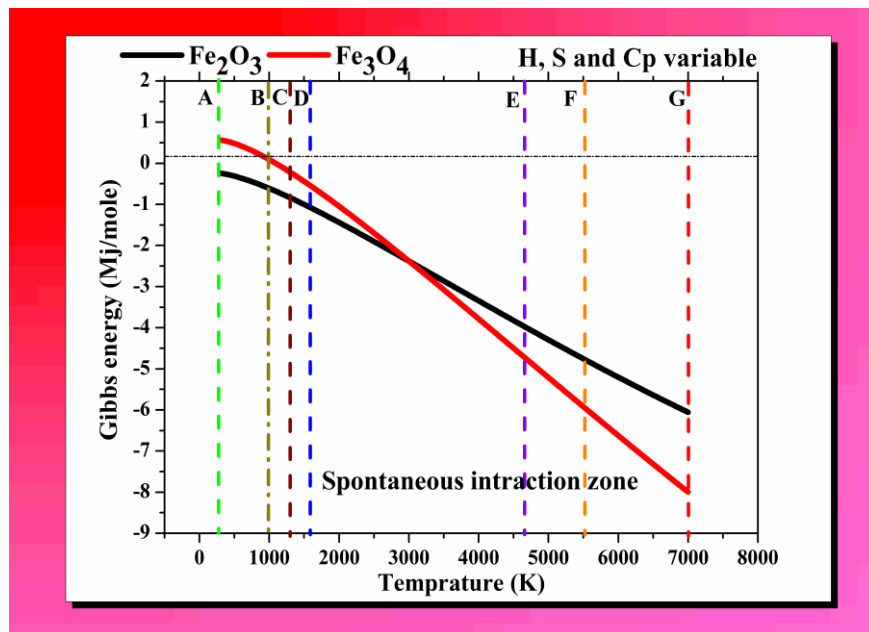


Figure (7) shows the change in the entropy of the reaction, when the heat capacity of the two reactions studied is constant when the temperature changes in the Earth's depths.

In the third case (see Figure (7)) the decrease is not initially linear, as linearity only appears starting from the beginning of the lower mantle of the Earth. Where the slope of change is estimated by 1.24 Mjoule/K for the

first reaction, while it is estimated at 1.82 Mjoule/K for the second reaction. That is, the decrease is faster for this last reaction, so the value of this energy for the two reactions is identical at the depth whose value is 1669.9 km and corresponding to the temperature estimated at 2990 K and located in the middle of the lower mantle of the Earth. After this depth, the energy values of the first reaction become higher than the energy values of the other reaction. It also appears from the same figure that the first reaction is always spontaneous for any depth in the Earth, while the second reaction becomes spontaneous only starting from the depth estimated at 77.89 km and corresponds to the estimated temperature value at 1092 K exactly at the boundary between the Earth's crust and the lithosphere region. In addition to this figure and the values recorded in Table (4), this energy changes in a range with a width of 5.81 Mjoule for the first reaction, while for the second reaction in a range with a width of 8.56 Mjoule. Also, the difference between the energy values between the two reactions is estimated at 0.81 Mjoule the surface of the Earth's crust, and is estimated at 1.94 Mjoule in the center of the Earth's interior.

IV- Conclusion:

Through this calculation we have reached; the reaction of producing Wüstite from the decomposition of Hematite always occurs starting from the Earth's surface, while the production of Wüstite from the decomposition of Magnetite occurs regardless of the case at different depths. It is in the Earth's crust close to the lithosphere region or at its beginning or in the middle of the Earth's lower mantle that appears in the case of the third coefficients not changing with temperature. With the production of this oxide remaining from these two decompositions at the rest of the Earth's depths. This means that the production of this oxide is more expected when decomposing Hematite, with a permanent production of oxygen regardless of the decomposition. Because this particular decomposition requires lower reaction enthalpy and entropy than the second decomposition, especially with increasing depth in the Earth. Although it requires less free energy, that is only when calculating based on the non-changes of the other three coefficients or their change together, especially before the darkness of the middle of the Earth's lower mantle.

In the future, this work can be developed by eliminating some of the assumptions made here, which could yield more accurate results than assuming constant pressure, which is not possible especially in the depths of the Earth's layers. Therefore, it is necessary to adopt a change in this thermodynamic parameter. Moreover, the search for other materials that produces this oxide, which may be found in the Earth's crust. Generalizing the study to other oxides important in the formation of the Earth's inner layers, such as MgO, CaO, BaO, NiO, and others.

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