

The thermodynamic properties of the upper continental crust: Exergy, Gibbs free Energy and Enthalpy

Alicia Valero¹, Antonio Valero¹ and Philippe Vieillard²

¹CIRCE. Centro de Investigación de Recursos y Consumos Energéticos
²HYDRASA, Faculté des Sciences, Université de Poitiers

Abstract: In this paper, the thermodynamic properties of the most abundant minerals of the upper continental crust are presented. For those substances whose thermodynamic properties are not listed in the literature, their enthalpy, Gibbs free energy and exergy are calculated with 12 different estimation methods presented in this paper, with associated errors ranging from 0 to 10%. Accordingly, the thermodynamic properties of the bulk continental crust are obtained. Finally, the chemical exergy of the continental crust is compared to the exergy of the concentrated mineral resources. The numbers obtained indicate that the chemical exergy of the crust is huge. However, only 0,001% of that amount can be effectively used by man.

Keywords: Exergy, Enthalpy, Gibbs Free Energy, Minerals.

1. Introduction

The upper continental crust is the reservoir of the main minerals and other natural resources useful for mankind. As stated in [1], a lot of effort has been placed in determining the chemical composition of the upper continental crust, but the mineralogical composition of it has been barely studied. This is due mainly to the complexity and heterogeneity of the earth's crust.

In this paper our final goal is to obtain the chemical exergy of the Earth's upper crust and to compare it with that of the concentrated minerals, i.e., with what we call mineral resources.

But for that purpose, knowing the chemical composition of the elements that compose the crust is not enough. We need to know the mineralogical composition of it. In [1], we obtained a first model of mineralogical composition of the crust. The latter will be used in this paper for obtaining the chemical exergy of the bulk upper crust.

2. Methodology

Assuming that the upper continental crust is composed by an ideal solution of substances, the average Enthalpy ($\Delta\bar{H}_f$), Gibbs free energy ($\Delta\bar{G}_f$) and Chemical Exergy (\bar{b}_{ch}) of each layer of the earth expressed as kJ/mole of atmosphere, hydrosphere or upper crust, are calculated as:

$$\Delta\bar{H}_f = \sum_{i=1}^m (x_i \cdot \Delta H_{fi}) \quad (1)$$

$$\Delta\bar{G}_f = \sum_{i=1}^m x_i \cdot (\Delta G_{fi} + \bar{R}T_0 \ln x_i) \quad (2)$$

$$\bar{b}_{ch} = \sum_{i=1}^m x_i \cdot (b_{chi} + \bar{R}T_0 \ln x_i) \quad (3)$$

Being x_i , molar fraction of the species composing each sphere of the earth, and ΔH_{fi} , ΔG_{fi} and b_{chi} , their enthalpy, Gibbs free energy and chemical exergy in kJ/mole, respectively.

The enthalpy and Gibbs free energy of the substances are obtained either through the literature or through the estimation methods explained in the next section.

The chemical exergy of the substance (b_{chi}) in kJ/mole is calculated with Eq. 4:

$$b_{chi} = \Delta G_f + \sum_j r_{j,i} b_{chj} \quad (4)$$

where b_{chj} is the standard chemical exergy of the elements that compose substance i . In our case we will use the chemical exergy of the elements obtained with an update of Szargut's R.E. [2] and published in [3].

The average enthalpy, Gibbs free energy and exergy of the continental crust, can be expressed in *mole/g* by substituting x_i with the molar fraction ξ_i for the i constituents of the sphere. Eq. 5 relates both properties through the molecular weight of the upper continental crust which was obtained in [1] as equal to $MW_{cr} = 157.7$ g/mole:

$$x_i = \xi_i \cdot MW_{cr} \quad (5)$$

3. Prediction of Enthalpy and Gibbs free energy of formation of minerals

The determination of the thermodynamic properties of the substances requires the knowledge of their corresponding enthalpies and Gibbs free energies of formation. Many of these have been already estimated through empirical and semi-empirical processes¹ and are tabulated. Comprehensive compilations of the thermodynamic properties of inorganic substances can be found in Faure [4], Wagman [5], Robie et al. [6], [7] or Weast et al. [8].

Unfortunately, not all the enthalpies and Gibbs free energies of the minerals that compose the earth's upper crust are recorded in the literature. Nevertheless, many of them can be predicted satisfactorily through different semi-empirical methods. In the next sections, the estimation methods of the thermodynamic properties used to obtain the standard enthalpy and Gibbs free energy of formation of the minerals will be provided.

3.1. Calculation of ΔH_f^0 or ΔG_f^0 from s^0

If either ΔH_f^0 or ΔG_f^0 and the entropy (s^0) of the mineral under consideration are available, the unknown property can be easily calculated applying Eq. 6.

$$\Delta G_f^0 = \Delta H_f^0 - T_0 \cdot \Delta S \quad (6)$$

Where the entropy change ΔS is calculated from the standard entropy of the mineral and its constituent elements in the standard state ($T_0 = 298.15$ K and 1 bar), as in Eq. 7:

$$\Delta S = s_{mineral}^0 - \sum s_{elements}^0 \quad (7)$$

Note that this procedure does not have associated any error, since it is based on the definition of ΔG_f .

¹Such as calorimetric or solubility measurements.

3.2. The ideal mixing model

An ideal solid solution of i components with x_i molar fractions obeys the equations:

$$\Delta H_m = 0 \quad (8)$$

$$\Delta G_m = +RT \sum x_i \ln x_i \quad (9)$$

Where ΔH_m and ΔG_m , are the enthalpy and Gibbs free energy of mixing. This means that the ideal mixing will take place without any heat loss or heat production. Moreover, the different cations will be fully interchangeable [9]. The enthalpy and Gibbs free energy of formation of the solid solution is calculated then with the following equations:

$$\Delta H_{f,solution}^0 = \sum_i x_i \Delta H_{f,i}^0 \quad (10)$$

$$\Delta G_{f,solution}^0 = \sum_i x_i \Delta G_{f,i}^0 + RT \sum x_i \ln x_i \quad (11)$$

The error associated to the assumption of the mineral as an ideal solid solution varies greatly with the mineral under consideration and decreases with the disorder among components. We will assume a maximum error of $\pm 1\%$.

3.3. Assuming ΔG_r and ΔH_r constant

3.3.1. Thermochemical approximations for sulfosalts and complex oxides

Craig and Barton [10] developed an approximation method for estimating the thermodynamic properties of sulfosalts in terms of mixtures of the simple sulfides. The ideal mixing model does not apply correctly to most sulfosalts, because the mixtures of layers are rather ordered. The modified ideal mixing model of Craig and Barton involves a mixing term (ΔG_m) in the estimation of the Gibbs free energy of formation of the sulfosalt per gram atom of S that is added to the weighted sum of free energies of the simple sulfides:

$$\Delta G_m = (1.2 \pm 0.8)(+RT \sum x_i \ln x_i) \quad (12)$$

The mixing term can be divided into two parts, one estimated from the crystal structure as an entropy change, and the reminder as a non-ideal term. The non-ideal term of this model was assumed to be constant for all sulfosalts. However, Vieillard [11]

showed that the properties of complex sulfides with respect to their simple sulfides are a function of the electronegativity difference between the cations of the sulfosalts.

The thermodynamic properties of sulfosalts (sfs) may then be calculated by adding a term (ΔH_r or ΔG_r) to the appropriately weighted sum of the enthalpies or free energies of the simple component sulfides:

$$\Delta H_{f,sfs} = \sum x_i \Delta H_{f,sulfides} + n_{S,sfs} \Delta H_r \quad (13)$$

$$\Delta G_{f,sfs} = \sum x_i \Delta G_{f,sulfides} + n_{S,sfs} \Delta G_r \quad (14)$$

The reaction term, which is analogous to the mixing term of Craig and Barton is associated to one atom of sulfur in the mineral ($n_{S,sfs}$) and is obtained from a sulfosalts for which its thermodynamic properties and those of its simple sulfides are known. The calculated reaction terms can be applied to a family of sulfosalts formed by the same cations and with partial element substitutions.

Vieillard et al. [11] demonstrated the analogy between the electronegativity scale of cations with respect to sulfur and to oxygen. They showed that the methodology of estimation of the thermodynamic properties of sulfosalts from simple sulfides can be equally applied to complex oxides able to be decomposed into simple oxides. As for sulfosalts, the reaction terms ΔH_r and ΔG_r (for this case denoted as ΔH_{ox} and ΔG_{ox}) should be obtained for an oxide of the same family of the mineral under analysis. The maximum error associated to this methodology is assumed to be $\pm 1\%$.

3.3.2. The method of corresponding states

Similarly, the ΔH_r and ΔG_r can be assumed to be constant in the substitution reaction of minerals A-x and B-x into A-y and B-y, if A-x and B-y are isomorphous. The associated error is assumed to be equal to the previous method, hence $\pm 1\%$.

3.4. The method of Chermak and Rimstidt for silicate minerals

The method proposed by Chermak and Rimstidt [12] predicts the thermodynamic properties (ΔG_f^0 and ΔH_f^0) of silicate minerals from the sum of polyhedral oxide and hydroxide contributions. The technique is based on the observation that silicate

minerals have been shown to act as a combination of basic polyhedral units. Chermak and Rimstidt determined by multiple linear regression, the contribution of $Al_2O_3^{[4]}$, $Al_2O_3^{[6]}$, $Al(OH)_3^{[6]}$, $SiO_2^{[4]}$, $MgO^{[6]}$, $Mg(OH)_2^{[6]}$, $CaO^{[6]}$, $CaO^{[8-z]}$, $Na_2O^{[6-8]}$, $K_2O^{[8-12]}$, H_2O , $FeO^{[6]}$, $Fe(OH)_2^{[6]}$ and $Fe_2O_3^{[6]}$ to the total ΔG_f^0 and ΔH_f^0 of a selected group of silicate minerals². The thermodynamic properties of the minerals are calculated with Eqs. 15 and 16:

$$\Delta H_f^0 = \sum x_i \cdot h_i \quad (15)$$

$$\Delta G_f^0 = \sum x_i \cdot g_i \quad (16)$$

Where x_i is the number of moles of the oxide or hydroxide per formula unit and h_i and g_i are the respective molar enthalpy and free energy contribution of 1 mole of each oxide or hydroxide component. The values of h_i and g_i for the different polyhedral components are listed in [12].

The errors associated to the estimated vs. experimentally measured values can reach $\pm 1\%$ for ΔG_f^0 and ΔH_f^0 , depending on the nature of the compounds. Note that this methodology can only be applied to those minerals able to be decomposed by the oxides and hydroxides mentioned before.

3.5. The ΔO^{-2} method

The linear additivity procedures based on the ΔO^{-2} parameter were developed by Yves Tardy and colleagues [13]. The parameter ΔO^{-2} , corresponds to the enthalpy $\Delta_H O^{-2}$ or Gibbs free energy $\Delta_G O^{-2}$ ³ of formation of a generic oxide $MO_x(c)$ from its aqueous ion, where z is the charge of the ion and x the number of oxygen atoms combined with one atom M in the oxide ($x = z/2$):

$$\Delta_H O^{-2} M^{z+} = \frac{1}{x} [\Delta H_f^0 MO_{x(c)} - \Delta H_f^0 M_{(aq)}^{z+}] \quad (17)$$

For hydroxides, silicates, phosphates, nitrates and carbonates involving two cations, it was found that the enthalpy and Gibbs free energy of formation of a given compound from its constituent oxides vary

²The brackets next to the chemical formulas of oxides and hydroxides indicate the coordination number of the polyhedral structure.

³The calculation of $\Delta_G O^{-2}$ is analogous to that of $\Delta_H O^{-2}$.

linearly with ΔO^{-2} and have the general expressions [14]:

$$\Delta H_{ox}^0 = \alpha_H \frac{n_i \cdot n_j}{n_i + n_j} [\Delta_H O^{2-} M_i^{z_i^+}(aq) - \Delta_H O^{2-} M_j^{z_j^+}(aq)] \quad (18)$$

Being ΔH_{ox}^0 ⁴:

$$\Delta H_{ox}^0[(M_i)_{n_i}(M_j)_{n_j}O_N] = \Delta H_f^0[(M_i)_{n_i}(M_j)_{n_j}O_N] - n_i \Delta H_f^0 M_i O_{x_i}(c) - n_j \Delta H_f^0 M_j O_{x_j}(c) \quad (19)$$

Where n_i and n_j are the numbers of oxygen ions linked, respectively, to the $M_i^{z_i^+}$ and $M_j^{z_j^+}$ cations; and N is the number of oxygens linked to the molecular structure of the double oxide ($N = x_i + x_j$). Parameters α_H and α_G are empirical coefficients variable from one family of compounds to another one (α_G is 0.84 for hydroxides, 1.01 for silicates, 1.15 for carbonates, 1.30 for nitrates, etc.).

Equation 18, yields a statistical deviation of 35 kJ/mole for the Gibbs free energy of formation and depends on the family of compounds. We will assume a maximum error associated to the ΔO^{2-} general method of $\pm 1\%$.

3.5.1. The ΔO^{-2} method for hydrated clay minerals and for phyllosilicates

Vieillard extended the methodology described above for the prediction of hydrated clay minerals [15] and for phyllosilicates [16].

The Gibbs free energy of formation of a hydrated clay mineral or a phyllosilicate composed by n_s cations located in different crystal sites and with $n_s(n_s - 1)/2$ interaction terms is calculated as:

$$\Delta G_f^0 = \sum_{i=1}^{i=n_s} (n_i) \Delta G_f^0(M_i O_{x_i}) + \Delta G_{ox}^0 \quad (20)$$

The Gibbs free energy of formation from the oxides ΔG_{ox}^0 is calculated with Eq. 21:

$$\Delta G_{ox}^0 = -N \left(\sum_{i=1}^{i=n_s-1} \sum_{j=i+1}^{j=n_s} X_i X_j (\Delta_G^{2-} M_i^{z_i^+}(clay) - \Delta_G^{2-} M_j^{z_j^+}(clay)) \right) \quad (21)$$

⁴The calculation of ΔG_{ox}^0 is analogous to that of ΔH_{ox}^0 .

where N is the total number of O atoms of all oxides; X_i and X_j are the molar fraction of oxygen related to the cations $M_i^{z_i^+}$ and $M_j^{z_j^+}$ in the individual oxides $M_i O_{x_i}$ and $M_j O_{x_j}$, respectively ($X_i = (1/N)(n_i x_i)$ and $X_j = (1/N)(n_j x_j)$). Parameters $M_i^{z_i^+}(clay)$ and $M_j^{z_j^+}(clay)$ characterize the electronegativity of cations $M_i^{z_i^+}$ and $M_j^{z_j^+}$ in a specific site and are calculated by minimizing the difference between experimental Gibbs free energies and calculated ones from constituent oxides. The predicted Gibbs free energy values showed an error between 0.0 and 0.6 %.

3.5.2. The ΔO^{-2} method for different compounds with the same cations

Tardy [14] showed that the Gibbs free energy of formation of a compound from its two constituent oxides calculated per one oxygen in the formula was a parabolic function of mean ΔO^{-2} compound. Subsequently, an expression for calculating the Gibbs free energy of formation of a compound C intermediate in composition to two compounds A and B , $A + B \rightarrow C$ was developed:

$$\Delta G_{ox,A+B \rightarrow C} = +\alpha (\Delta_G O^{2-} M_i^{z_i^+} - \Delta_G O^{2-} M_j^{z_j^+}) n_C (X_i^C - X_i^A)(X_i^C - X_i^B) \quad (22)$$

where n_c designates the total number of oxygens of the compound C and X_i^A , X_i^B , X_i^C the mole fractions of oxygen that balance cation $M_i^{z_i^+}$ in compounds A , B , and C and α the correlation parameter for a given class of compounds.

3.6. Assuming ΔS_r zero

Helgeson et al. [17] showed that the entropy of formation of mineral a certain mineral can be determined, assuming that the entropy of the reaction involved in the formation of the mineral is zero (Helgeson's algorithm). Helgeson algorithm is useful when either ΔG_f or ΔH_f are known. Once the entropy of the mineral is known, ΔG_f (or ΔH_f) can be calculated with ΔH_f (or ΔG_f) through Eq. 6. The error associated to this approximation is up to 5%.

3.7. Assuming ΔG_r and ΔH_r zero

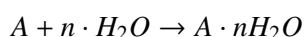
3.7.1. The element substitution method

In some cases, thermodynamic properties are available for a certain mineral (A), belonging to the same

family of the substance under consideration (B), but with partial element substitutions. In such a case, the ΔH_f^0 and ΔG_f^0 of mineral B can be calculated from mineral A , assuming that the reaction enthalpy or free energy of formation of mineral B from A is zero. This approximation increases with the magnitude of substitution and may yield to associated errors of up to 5%, although it rarely exceeds $\pm 2\%$.

3.7.2. The addition method for hydrated minerals

Hydrated minerals have the ability to absorb water molecules, forming part of their crystal structure:



Usually, thermodynamic properties are available for the non-hydrated mineral. But the enthalpy and Gibbs free energy of formation of the hydrated substance can be estimated by addition of the hydration enthalpy and Gibbs free energy ΔG_{hydr}^0 or ΔH_{hydr}^0 to those of the dehydrated substance, as in Eqs. 23.

$$\begin{aligned} \Delta H_{f,A \cdot nH_2O}^0 &= \Delta H_{f,A}^0 + n \cdot \Delta H_{hydr,A}^0 \\ \Delta G_{f,A \cdot nH_2O}^0 &= \Delta G_{f,A}^0 + n \cdot \Delta G_{hydr,A}^0 \end{aligned} \quad (23)$$

If ΔG_{hydr}^0 and ΔH_{hydr}^0 are not available, one can assume that the enthalpy and Gibbs free energy of the hydration reaction are zero (as in section 3.7.1.). And hence, the properties of the liquid water molecules contained in the hydrated substance must be added in place of ΔG_{hydr}^0 and ΔH_{hydr}^0 . This is not rigorously exact, as demonstrated by Vieillard and Jenkins ([18], [19], [20]) and the error associated depends on the nature of the dehydrated component⁵. We will assume an associated error of $\pm 5\%$, although it rarely exceeds $\pm 2\%$.

3.7.3. The decomposition method

If none of the previously described methods can be applied, the thermodynamic properties of a certain mineral can be estimated as the last resort by decomposing it into its major constituents for which the enthalpy and Gibbs free energy of formation are known. It will be assumed that the energy of reaction of the constituents to form the mineral under consideration is zero. The error associated to this

⁵This methodology is not applied for hydrated clay minerals and phyllosilicates. In those cases, the ΔO^{2-} method is applied.

methodology is significantly greater than with the substitution and addition methods, since in this case we are not dealing with partial substitutions or additions of a known mineral, but with the formation of a completely new mineral from its building blocks. The mineral under analysis will be decomposed into its most complex compounds (usually double silicates). If this is not possible, most minerals can be decomposed into its simple oxides, sulfides, carbonates, etc. We will assume that the decomposition method throws an error of up to 10%.

3.8. Summary of the methodologies

The described methodologies in the previous sections, will be used for calculating the thermodynamic properties of the most abundant minerals in the earth's upper crust. Each methodology is given a number so as to specify in the next section, which methodology has been used for determining the enthalpy or free energy of formation of the minerals (see table 1). Additionally, the assumed maximum errors associated to the estimation methods ($\pm \varepsilon$) are given.

Table 1: Summary of the methodologies used to predict the thermodynamic properties of minerals

Method	Nr.	$\pm \varepsilon$, %
Calculation of ΔH_f^0 or ΔG_f^0 from s^0	1	0
The ideal mixing model	2	1
Thermochemical approximations for sulfosalts and complex oxides	3	1
The method of corresponding states	4	1
The method of Chermak and Rimstidt for silicate minerals	5	1
The ΔO^{-2} method	6	1
The ΔO^{-2} method for hydrated clay minerals and for phyllosilicates	7	0.6
The ΔO^{-2} method for different compounds with the same cations	8	1
Assuming ΔS_r zero	9	5
The element substitution method	10	5
The addition method for hydrated minerals	11	5
The decomposition method	12	10

4. Results

Table 3 shows the the thermodynamic properties of the 291 main minerals included in the crust. About a half of the properties (159) were compiled directly from the literature. The remaining were obtained with the 12 different estimation methods described in [21]. From the latter, 18 minerals were calculated

without committing any associated error. Five minerals were estimated committing a maximum error of $\epsilon < 0.6\%$. Thirty-eight minerals were estimated with an error smaller than 1%, 20 substances with $\epsilon < 5\%$, and 44 minerals with $\epsilon < 10\%$. Only the properties of 6 minerals: iridium, osmium, nickel, polixene, sylvanite and yttrialite were not able to be estimated. Additionally, the enthalpy of formation of gersdorffite and the Gibbs free energy of smaltite are missing. Nevertheless, all together account for only $3.5 \times 10^{-6}\%$ of the continental crust. It should be pointed out that the R.E. generates some negative exergies of the minerals. This is because we chose our R.E. based on Szargut's criterion of partial stability. According to this, among a group of reasonable abundant substances, the most stable will be chosen if they also satisfy the "earth similarity criterion". This criterium is different from that of [22] or [23], where complete stability was assumed. As a consequence, the latter R.E. do not generate any negative exergies, but the resulting environment is completely different from that of the current earth. Our chosen R.E. obeys in principle the "earth similarity criterion", but does generate some negative exergies. Hence, this leads us to question the methodology used for establishing the R.E.

4.1. The chemical exergy of the earth

With these results, we can now calculate the average standard enthalpy, Gibbs free energy and chemical exergy of the upper continental crust with Eqs. 1-3:

$$\begin{aligned}(\Delta\bar{H}_f^0)_{cr} &= -1959.96 \text{ kJ/mole} \\(\Delta\bar{G}_f^0)_{cr} &= -1841.10 \text{ kJ/mole} \\(\bar{b}_{ch}^0)_{cr} &= 366.56 \text{ kJ/mole}\end{aligned}$$

For the calculation of the absolute exergy of the continental crust, we require information about its total mass. According to [24], the earth has a mass of around 5.98×10^{24} kg. The earth's relative mass proportions of each of the earth's spheres are according to [25]: core (35.5%), mantle (67%), oceanic crust (0.072%), continental crust (0.36%), hydrosphere (0.023%) and atmosphere (0.842 ppm). The upper layer of the crust constitutes a mass of around 50% of the whole continental crust [26]. With this information we can obtain a first approximation of the

exergy of the upper continental crust (see table 2). It has been assumed that there is no mixing among the considered layers and hence the Gibbs free energy and exergy of the mixture is zero.

Table 2: Exergy of the bulk upper crust

Mass, kg	MW, g/mole	\bar{b}_{ch}^0 , kJ/mole	\bar{B}_{ch}^0 , Gtoe
1.08E+22	157.7	366.56	5.97E+08

Of course these are very rough numbers, and are subject to ulterior updates, especially when a more appropriate R.E. is found. But they are good enough, for providing an order of magnitude of the chemical exergy of our planet.

In [27] we carried out an inventory of the exergy resources of the Earth. For the case of non renewable resources, including nuclear energy, fossil fuels and non-fuel minerals, the estimation of the available exergy on Earth obtained was at least around 115000 Gtoe, from which 65% come from the not yet technologically developed fusion of deuterium and tritium. The potential exergy use of non-renewable resources was around 6000 Gtoe. Considering these figures, we can now state that the non-renewable available resources contribute to a very small fraction of the total chemical exergy of the earth: less than 0.02%. The exergy of conventional fossil fuels and non energy mineral resources, constitute only 0.001% of the upper continental crust's chemical exergy.

5. Conclusions

In this paper, the standard thermodynamic properties of the main constituents of the upper Earth's crust have been provided for the first time. That is the standard enthalpy, Gibbs free energy and chemical exergy of more than 330 natural substances.

The enthalpies and Gibbs free energies, have been obtained either from the literature, or have been calculated with the 12 estimation methods described in this paper. The exergy of the substances has been calculated with the chemical exergies of the elements, generated with a R.E. based on Szargut's methodology.

Despite of the limitations of the R.E. pointed out, it still constitutes a tool for obtaining chemical exergies. Since the mass of the earth and of its spheres is

known, we were able to calculate the absolute chemical exergy of the upper continental crust: 6.0×10^8 Gtoe. Obviously the numbers are very rough, and are subject to ulterior updates, but they are good enough, for providing an order of magnitude of the huge chemical wealth of our planet.

The wealth of our planet is enormous, but man can only take advantage of a very small part of it: the resources. With current technology, it is impossible to use the chemical exergy of dispersed substances. Non-renewable resources are considered as such, because they represent a stock of concentrated chemical exergy. Therefore, the earth's 6.0×10^8 Gtoe of chemical exergy constitutes nowadays a useless reservoir of exergy. Consequently, we should resign ourselves with a maximum of only 0.02% of that amount.

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Table 3: Thermodynamic properties of the upper continental crust

Mineral	Formula	ϵ_r , mole/g	ΔH_f^0 kJ/mole	ΔG_f^0 kJ/mole	Reference	$\pm\epsilon$, %	$h_{0,i}$, kJ/mole
Quartz	SiO_2	3.81E-03	-911.6	-857.2	[4]		1.0
Albite	$NaAlSi_3O_8$	5.14E-04	-3927.6	-3704.5	[4]		4.8
Oligoclase	$Na_{0.8}Ca_{0.2}Al_{1.2}Si_{2.8}O_8$	4.49E-04	-796.0	-750.9	[4]		3023.9
Orthoclase/ K-feldspar	$KAlSi_3O_8$	4.22E-04	-3977.5	-3752.1	[4]	0	-12.8
Andesite	$Na_{0.6}Ca_{0.4}Al_{1.4}Si_{2.6}O_8$	2.03E-04	-808.9	-763.7	[4]		3076.6
Opal	$SiO_2 \cdot 0.5H_2O$	1.42E-04	-1044.5	-967.9	[4]	5	9.3
Augite	$Ca_{0.9}Na_{0.1}Mg_{0.9}Fe_{0.2}^{2+}Al_{0.4}Ti_{0.1}Si_{1.9}O_6$	1.27E-04	-3201.5	-3026.8	[6]		-446.9
Labradorite	$Na_{0.5}Ca_{0.5}Al_{1.5}Si_{2.5}O_8$	9.25E-05	-815.0	-769.8	[4]		3103.2
Biotite	$K(Mg_{2.5}Fe_{0.5})(Si_{3.5}Al_{0.5})O_{10}(OH)_{1.75}F_{0.25}$	8.80E-05	-6079.4	-5706.7	[4]	1	78.6
Calcite	$CaCO_3$	8.00E-05	-1207.7	-1129.0	[4]	1	325.2
Hydromuscovite/ Illite	$K_0.6(H_3O)_{0.4}Al_2Mg_{0.4}Fe_{0.1}^{2+}Si_{3.5}O_{10}(OH)_2$	7.73E-05	-5886.2	-5499.1	[4]	1	11.0
Sillimanite	Al_2SiO_5	6.15E-05	-2587.4	-2441.0	[4]		11.7
Paragonite	$NaAl_3Si_3O_{10}(OH)_2$	4.95E-05	-5932.5	-5557.6	[4]		-15.7
Nontonrite	$Na_{0.3}Fe_{0.3}^{2+}(Si_{3.7}Al_{0.3})O_{10}(OH)_2 \cdot 4(H_2O)$	3.88E-05	-6841.0	-5447.7	[4]	0.6	738.2
Magnetite	$Fe_3^{2+}Fe^{2+}O_4$	3.43E-05	-1118.3	-1015.9	[4]		122.6
Kaolinite	$Al_2Si_2O_5(OH)_4$	3.24E-05	-4117.7	-3796.0	[4]		-9.0
Ilmenite	$Fe^{2+}TiO_3$	3.10E-05	-1237.2	-1163.5	[4]		123.7
Diopside	$AlO(OH)$	2.95E-05	-998.1	-917.6	[4]		-1.3
Hornblende-Fe	$Ca_2Fe^{2+}Al_0.75Fe_{0.25}^{3+}(Si_{7.7}Al_{0.22})OH_2$	2.78E-05	-10976.4	-10303.7	[4]		398.5
Muscovite	$KAl_2Si_3O_{10}(OH)_{1.8}F_{0.2}$	2.54E-05	-5991.3	-5616.6	[4]	1	-13.1
Titanite	$CaTiSiO_5$	2.28E-05	-2597.1	-2455.1	[4]	0	37.2
Almandine	$Fe_2^{2+}Al_2(SiO_4)_3$	2.09E-05	-5305.5	-4969.8	[4]		335.7
Graphite	C	2.01E-05	0.0	-7788.2	[4]		410.3
Rhpidolite	$(Mg_{0.75}Fe_{1.25}Al)(Si_{13}AlO_{10})(OH)_2(OH)_6$	2.01E-05	-8429.2	-7788.2	[4]	0.6	175.2
Epidote	$Ca_2Fe^{3+}Al_2(SiO_4)_3(OH)$	1.87E-05	-6466.1	-6076.3	[4]		43.1
C. ogg	C	1.84E-05	N.A.	N.A.	[4]		N.A.
Hydragillite/ Gibbsite	$Al(OH)_3$	1.77E-05	-1282.2	-1155.8	[4]		-1.4
Diopside	$CaMgSi_2O_6$	1.40E-05	-3031.2	-3026.3	[4]		47.4
Beidellite	$Na_{0.33}Al_{0.33}Si_{3.67}O_{10}(OH)_2$	1.39E-05	-5691.6	-5317.2	[4]		39.4
Ankerite	$CaFe_{0.6}^{2+}Mg_{0.3}Mn_{0.1}^{2+}(CO_3)_2$	1.36E-05	-2076.8	-1923.1	[6]	10	96.6
Aegirine	$NaFe^{3+}Si_2O_6$	1.32E-05	-2585.5	-2417.2	[6]		16.5
Andalusite	Al_2SiO_5	1.25E-05	-2590.4	-2443.0	[4]		9.7
Hyperstene	$MgFe^{2+}Si_2O_6$	1.17E-05	-2757.4	-2594.6	[4]		132.2
Goethite	$Fe^{3+}O(OH)$	1.17E-05	-559.4	-489.2	[4]		9.7
Halite	$NaCl$	1.01E-05	-386.3	-384.4	[4]		14.3
Boehmite	$AlO(OH)$	9.65E-06	-988.1	-914.1	[4]		2.2
Bytownite	$Na_{0.2}Ca_{0.8}Al_{1.8}Si_{2.2}O_8$	9.08E-06	-4186.8	-3960.7	[4]		10.5
Phosphate rock	$Ca_3(PO_4)_2$	8.99E-06	-3886.6	-3878.2	[4]		32.4
Natrofite	$Na_2Al_2Si_3O_{10} \cdot 2(H_2O)$	7.82E-06	-5722.1	-5316.6	[4]		3.8
Dolomite	$CaMg(CO_3)_2$	7.63E-06	-2327.9	-2167.9	[4]		18.0
Clinochlore	$Mg_3.75Fe_{1.25}Al_2Si_3O_{10}(OH)_8$	7.33E-06	-8435.5	-7796.6	[4]	1	166.8
Montmorillonite	$Na_{0.165}Ca_{0.084}Al_{2.33}Si_{3.67}O_{10}(OH)_2$	6.52E-06	-5523.8	-5354.5	[4]	1	39.6
Lawsonite	$CaAl_2Si_2O_7(OH)_2 \cdot H_2O$	6.36E-06	-4812.8	-4510.6	[4]	5	2.2
Riebeckite	$Na_2Fe_3^{2+}Fe_2^{3+}(Si_8O_{22})(OH)_2$	6.14E-06	-10087.1	-9399.5	[4]	0	318.9
Hematite	Fe_2O_3	6.05E-06	-826.1	-742.2	[4]		17.4
Sepiolite	$Mg_4Si_6O_{15}(OH)_2 \cdot 6(H_2O)$	5.67E-06	-10123.7	-9257.8	[4]		1284.5
Hydrobiotite	$(K_{0.5}Ca_{0.1})(Mg_{2.3}Fe_{0.8}^{3+}Al_{0.1})(Si_{2.8}Al_{1.2})O_{10}(OH)_{1.8}F_{0.2} \cdot 3(H_2O)$	5.26E-06	-7362.2	-6238.9	[4]	5	46.2
Ulvöspinel	$TiFe_2^{2+}O_4$	5.21E-06	-1489.4	-1392.9	[4]	10	273.1
Diene/Kyanite	Al_2SiO_5	4.37E-06	-2593.7	-2442.0	[4]		10.7
Cummingtonite	$Mg_7(Si_8O_{22})(OH)_2$	3.73E-06	-12070.0	-11343.0	[6]		181.6
Glaucophane	$Na_7(Mg_3Al_2)Si_8O_{22}(OH)_2$	3.65E-06	-12080.6	-11346.7	[4]		-78.8
Celestine	$SrSO_4$	3.65E-06	-1454.1	-1341.6	[4]		32.4
Prehnite	$Ca_2Al_2Si_3O_{10}(OH)_2$	3.58E-06	-6197.3	-5823.0	[4]		35.7
Rutile	TiO_2	3.41E-06	-945.4	-890.1	[4]		18.3
Barite	$BaSO_4$	3.04E-06	-1470.4	-1361.9	[4]		18.8
Niter	KNO_3	2.96E-06	-495.0	-395.2	[4]		-22.3
Nitratine	$NaNO_3$	2.96E-06	-468.2	-367.1	[4]		-24.2
Pennine	$(Mg_{0.75}Fe_{1.25}Al)(Si_{13}AlO_{10})(OH)_2(OH)_6$	2.87E-06	-8429.2	-7788.2	[4]	0.6	175.2

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Table 3: Thermodynamic properties of the upper continental crust. – continued from previous page.

Mineral	Formula	ξ_i , mole/g	$\Delta H_{f,i}^\circ$, kJ/mole	$\Delta G_{f,i}^\circ$, kJ/mole	Reference	$\pm \epsilon$, %	$b_{th,i}$, kJ/mole
Actinolite	$Ca_2Mg_3Fe_2Si_8O_{22}(OH)_2$	2.82E-06	-11519.4	-10801.5		1	405.9
Pyrite	FeS_2	2.75E-06	-175.0	-163.3	[4]		1428.1
Sandine	$K_0.75Na_{0.25}AlSi_3O_8$	2.67E-06	-3860.7	-3715.9		1	15.9
Hastingsite	$NaCa_2Fe_2^{3+}Fe^{2+}(Si_{16}Al_2O_{22})(OH)_2$	2.60E-06	-11926.3	-11343.4	[28]		289.2
Ferrosillite	$Fe_2^{2+}MgSi_2O_6$	2.32E-06	-2757.4	-2594.6	[4]		132.2
Zircon	$ZrSiO_4$	2.11E-06	-2034.8	-1919.5	[4]		20.0
Siderite	$Fe^{2+}CO_3$	2.08E-06	-742.3	-671.1	[4]		122.0
Spodumene	$LiAlSi_2O_6$	2.06E-06	-3056.8	-2882.9	[4]		24.6
Pigeonite	$Mg_{1.35}Fe_{0.55}Ca_{0.1}(Si_2O_6)$	1.99E-06	-1535.4	-1448.8	[4]		1401.1
Leucocane	$CaTiSi_2O_5$	1.90E-06	-2591.6	-2454.8	[4]		37.5
Pyrrhotite	$Fe^{2+}S$	1.79E-06	-105.5	-100.5	[4]		883.6
Leptodimela/Annite	$KFe_{2.5}^{2+}Mg_{0.5}Fe_{0.75}^{3+}Al_{0.25}Si_3O_{10}(OH)_2$	1.78E-06	-4995.0	-4642.3		1	284.8
Bronzite	$MgFe_2Si_2O_6$	1.77E-06	-2753.4	-2585.3		0	141.5
Anhydrite	$CaSO_4$	1.73E-06	-1435.1	-1322.7	[4]		16.3
Serpentine	$Mg_3Si_2O_5(OH)_4$	1.64E-06	-4363.4	-4035.4		0	51.9
Olivine	$Mg_{1.6}Fe_{0.4}SiO_4(SiO_4)$	1.53E-06	-2083.3	-1925.0		1	95.3
Enstatite	$Mg_2Si_2O_6$	1.39E-06	-3055.5	-2919.9		1	59.6
Corundum	Al_2O_3	1.20E-06	-1668.9	-1563.0	[4]		31.5
Thuringite-Chamosite	$(Fe_3Mg_2Fe_0.5^{3+}Al_0.5^{3+})(Si_3AlO_{10}(OH)_2)$	1.14E-06	-7596.0	-6981.9		0.6	-389.8
Nepuntite	$KNa_2LiFe_{1.5}^{2+}Mn_{0.5}^{2+}Ti_2Si_8O_{24}$	1.10E-06	-10724.6	-10061.3		10	868.9
Sphalerite	ZnS	1.02E-06	-206.1	-201.4	[4]		744.9
Analcime	$Na_4Al_3Si_3O_{12}(H_2O)$	1.01E-06	-3310.2	-3088.5	[4]		0.8
Anorthite	$CaAl_2Si_2O_8$	9.90E-07	-4274.4	-4021.0	[4]		15.6
Rhodochrosite	$MnCO_3$	9.48E-07	-894.7	-817.1	[4]		83.8
Chromite	$Fe^{2+}Cr_2O_4$	8.83E-07	-1445.7	-1358.4	[4]		195.1
Gypsum	$CaSO_4 \cdot 2H_2O$	7.96E-07	-2024.0	-1798.6	[4]		16.6
Pyrrusum	$Ca_2(PO_4)_3(OH)_{0.33}Fe_{0.33}Ca_{0.33}$	7.91E-07	-6773.4	-6386.9	[4]		-23.2
Apatite	$Fe^{2+}Al_6Si_4O_{23}(OH)_2$	7.68E-07	-12066.8	-11215.6	[4]		269.1
Staurolite	$Mg_3Si_4O_{10}(OH)_2$	7.67E-07	-5907.2	-5543.0	[4]		22.6
Talc	$CaCO_3$	7.64E-07	-1207.9	-1128.6	[4]		11.4
Aragonite	$Ca_2Al_3(SiO_4)_3(OH)$	7.51E-07	-6883.9	-6483.9	[4]		53.0
Clinozoisite	$Mg_3Si_4O_{10}(OH)_2 \cdot 2(H_2O)$	6.78E-07	-7018.8	-5957.2	[4]		1717.4
Vermiculite	$Mn_2^{2+}(SiO_4)$	6.30E-07	-1733.3	-1632.1	[4]		199.3
Tephroite	$NaCa_2Al_5Si_5O_{20} \cdot 6H_2O$	6.19E-07	-12413.7	-11543.9		1	-49.1
Thomsonite	$Ca_2Al_3Si_3O_{12}(OH)$	5.68E-07	-6883.9	-5416.5	[4]		1120.4
Zoisite	MnO_2	5.64E-07	-520.4	-465.2	[4]		23.4
Pyrolusite	TiO_2	5.59E-07	-940.4	-883.7	[4]		24.7
Anatase	B_2O_3	5.10E-07	-2569.1	-2347.2		1	2103.1
Psilomelane	$Na_0.75K_{0.25}Al(SiO_4)$	5.09E-07	-2087.6	-1972.4		1	28.1
Nepheline	Mg_2SiO_4	4.95E-07	-2175.5	-2057.8	[4]		63.6
Forsterite	$NaAlO_3Fe_0.3^{3+}(Si_2O_6)$	4.78E-07	-2990.4	-2812.1		1	-2.7
Jadeite	$Mn_2 + 3Al_2Si_2O_7$	4.77E-07	-5646.3	-5326.3	[29]		302.6
Spessartine	$Ca_0.5Li_{0.25}Na_{0.25}Th_{0.05}(PO_4)$	4.29E-07	-2074.0	-1943.3		10	-43.3
Monazite (Ce)	$Ca_2Mg_5Si_8O_{22}(OH)_2$	4.28E-07	-12367.8	-11639.3	[4]		73.7
Tremolite	$Na_2Mg_2Fe^{2+}Al_2(Si_8O_{22})(OH)_2$	4.06E-07	-11600.3	-10925.8		1	133.0
Crossite	$Mn^{2+}Mn^{3+}SiO_2$	4.06E-07	-4260.0	-3944.7	[6]		325.8
Braunite	$CaFeS_2$	3.62E-07	-194.6	-195.1	[6]		1330.3
Chalcopyrite	H_3BO_3	3.60E-07	-1095.1	-969.0	[4]		19.7
Sassolite	$MgCO_3$	3.58E-07	-1114.1	-1030.2	[4]		15.6
Magnesite	$Ti_{0.7}Nb_{0.15}Fe_{0.22}^{2+}O_2$	3.22E-07	-864.6	-813.2		1	45.5
Ilmenorutile	$BaCO_3$	3.04E-07	-1217.1	-1137.6	[4]		44.1
Witherite	$K_0.8Fe_8Al_{0.8}SSi_{11.1}O_{21}(OH)8 \cdot 6H_2O$	2.77E-07	-16655.5	-15197.0		0	5459.7
Stübelmelane	$CaFe^{2+}Si_2O_6$	2.75E-07	-284.4	-267.1	[4]		8651.4
Hedenbergite	$B_{0.8}Pb_{0.2}Na_{0.125}Fe_{1.3}Al_{0.25}Si_{10.1}Mn^{2+}Mg^{2+}O_{16}$	2.63E-07	-4733.3	-4330.4	[4]		288.3
Hollandite	$Fe_2^{2+}SiO_4$	2.54E-07	-1480.9	-1369.2	[4]		246.6
Fayalite	$Mn^{2+}SiO_3$	2.32E-07	-1321.6	-1243.1	[4]		101.7
Rhodonite	SiO_2	2.06E-07	-910.1	-855.5	[4]		2.7
Chrosomalite	$Ca_2MgAl_2(SiO_4)(Si_2O_7)(OH)_2 \cdot H_2O$	1.89E-07	-7148.6	-6672.5		1	57.9
Pumpellyite							

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Table 3: Thermodynamic properties of the upper continental crust. – continued from previous page.

Mineral	Formula	ξ_r , mole/g	ΔH_f^0 , kJ/mole	ΔG_f^0 , kJ/mole	Reference	$\pm\epsilon$, %	h_{01}^+ , kJ/mole
Phlogopite	$KMg_3AlSi_3O_{10}F(OH)$	1.58E-07	-6292.8	-5902.2		1	128.1
Manganite	$MnO(OH)$	1.55E-07	-622.4	-557.3		10	49.4
Fluorite	CaF_2	1.44E-07	-1220.5	-1168.1	[4]		111.9
Amblygonite	$Li_{0.75}Na_{0.25}Al(PO_4)F_{0.75}(OH)_{0.25}$	1.29E-07	-307.1	-282.7	[29]	10	1992.6
Vesuvianite	$Ca_{10}Mg_2Al_4(SiO_4)_5(Si_2O_7)_2(OH)_4$	1.20E-07	-12175.8	-119948.7			219.0
Jacobsite	$Mn_2^{2+}Fe_2^{3+}Mg^{2+}Fe^{3+}Mn_3^{2+}O_4$	1.20E-07	-1237.4	-1137.5		5	711.5
Bastnaesite	$La(CO_3)F$	1.16E-07	-1660.9	-1527.8		5	160.8
Arfvedsonite	$Na_3Fe_4^{2+}Fe^{3+}(Si_8O_{22})(OH)_2$	1.09E-07	-11926.3	-11201.5	[28]		-1146.5
Spinel	$MgAl_2O_4$	1.07E-07	-2281.0	-2172.5	[4]		53.6
Lepidolite	$KLi_2AlSi_4O_{10}F(OH)$	1.03E-07	-6003.2	-5654.7		1	126.7
Cordierite	$Mg_2Al_2Si_5O_{18}$	9.52E-08	-9114.7	-8603.9	[4]		139.2
Kernite	$Na_2O \cdot 2H_2O_2 \cdot 4H_2O$	8.99E-08	-4104.9	-3713.1		5	440.8
Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$	8.93E-08	-5632.5	-5257.6			7.6
Francolite	$Ca_5(PO_4)_2 \cdot 6H_2O$	8.68E-08	-5984.4	-5698.1		1	714.3
Orthite - Allamite	$Ca(C_{0.4}C_{0.2}Ca_{0.2}Fe_{0.133})(Al_2Fe^{3+}Si_3O_{12}(OH))$	7.81E-08	-6481.6	-6055.4		1	32.3
Pentlandite	$Fe_2^{2+}Ni_4S_8$	7.44E-08	-778.3	-766.2		10	6833.9
Ulexite	$NaCa(B_5O_6(OH)_2) \cdot 5H_2O$	7.19E-08	-6762.2	-6151.5		0	2855.3
Scapolite - Marialite	$Na_4Al_3Si_9O_{24}Cl$	6.34E-08	-12197.4	-11504.2		0	22.5
Chloritoid	$Fe^{2+}_2Mg_6Mn^{2+}_2Al_4Si_{12}O_{40}(OH)_4$	6.18E-08	-6606.9	-6152.6		1	159.8
Pollucite	$Ca_5Na_{0.2}Rb_{0.1}Al_6O_9Si_2O_6 \cdot (H_2O)$	6.14E-08	-3297.1	-3074.2		10	10.0
Colmanite	$Ca_2B_6O_{11} \cdot 5H_2O$	5.99E-08	-6949.7	-6277.0		5	-796.8
Beryl	$Be_3Al_2Si_6O_{18}$	5.99E-08	-9006.5	-8500.4		0	56.9
Marcasite	FeS_2	5.24E-08	-154.9	-156.6	[8]		1434.8
Grossular	$Ca_3Al_2(SiO_4)_3$	4.62E-08	-6631.1	-6281.0	[4]		65.4
Vaesite	NiS_2	4.23E-08	-134.2	-126.4	[30]		1320.6
Gedrite	$Mg_5Al_2(Si_6Al_5O_{22})(OH)_2$	4.12E-08	-12319.7	-11584.2		0	149.9
Tourmaline - Schorl	$NaFe_3^{2+}Al_6(BO_3)_3Si_6O_{18}(OH)_4$	4.09E-08	-14401.4	-13453.5		0	377.6
Wollastonite	$CaSiO_3$	4.08E-08	-1631.6	-1550.9	[4]		33.1
Clementite	$Fe^{2+}_2Mg_{1.5}AlFe^{3+}Si_3AlO_{12}(OH)_6$	3.81E-08	-7657.8	-7043.1		1	504.6
Cryptomelane	$K_8(Mn^{4+}_2Mn^{2+}_5)O_{16}$	3.09E-08	-3743.6	-3432.2		1	3409.1
Kieserite	$MgSO_4 \cdot (H_2O)$	3.06E-08	-1602.1	-1428.7	[5]		54.2
Arsenopyrite	$FeAsS$	2.89E-08	-41.9	-50.2	[4]		1428.0
Galena	PbS	2.79E-08	-100.5	-95.9	[4]		743.6
Murmanite	$Na_4Ti_{3.6}Nb_{0.4}(Si_2O_7)_2O_4 \cdot 4(H_2O)$	2.78E-08	-9804.0	-9096.6	[4]	10	354.0
Sylvite	KCl	2.74E-08	-437.0	-410.2	[4]		18.5
Brcite	$Mg(OH)_2$	2.71E-08	-925.9	-834.8	[4]		34.9
Anthophyllite	$Mg_7Si_8O_{22}(OH)_2$	2.67E-08	-12094.6	-11396.0	[4]		128.6
Ferrocolumbite	$Fe^{2+}_2Nb_2O_6$	2.40E-08	-2172.8	-2018.6		10	170.5
Covellite	CuS	2.27E-08	-53.2	-53.6	[4]		687.7
Vermadite	$Mn_{0.6}^{2+}Fe_{0.2}^{3+}Cu_{0.2}Nb_{0.1}O_{1.5}(OH)_{0.5} \cdot 1.4(H_2O)$	2.18E-08	-637.8	-571.4		1	393.5
Thortite	TiS_2O_4	2.13E-08	-2160.5	-2048.8		5	27.8
Nickeline	$NiAs$	2.04E-08	N.A.	N.A.			N.A.
Suphirine	$Mg_4Al_6S_{11}O_{20}$	2.04E-08	-10563.3	-9962.9	[4]		2366.3
Andradite	$Ca_3Fe^{2+}(SiO_4)_3$	1.96E-08	-5764.4	-5419.4	[4]		92.1
Chrysoberyl	$BeAl_2O_4$	1.80E-08	-2302.3	-2178.2	[4]		20.9
Cassiterite	SnO_2	1.73E-08	-581.1	-519.6	[4]		32.0
Violarite	$Fe^{2+}_2Ni_2S_4$	1.72E-08	-378.0	-368.9		1	2902.0
Todorokite	$Na_2Mn^{2+}Mn^{3+}O_{12} \cdot 3H_2O$	1.34E-08	-4033.7	-3576.5		1	742.6
Cubanite	$CuFe_2S_3$	1.33E-08	-293.7	-302.8		1	2406.7
Topaz	$Al_2(SiO_4)F_{11}(OH)_9$	1.29E-08	-3044.4	-2875.2		5	-11.4
Glaucophane	$(K_{0.6}Na_{0.05})(Fe^{2+}_3Mg_{0.4}Fe^{3+}_{0.2}Al_{0.2}O_{10}(OH)_2)$	1.21E-08	-5150.3	-4785.6		0.6	52.1
Garnierite	$(Ni_2Mg)Si_2O_5(OH)_4$	1.18E-08	-3494.6	-3267.1		1	25.9
Molybdenite	MoS_2	1.14E-08	-271.8	-262.8	[6]		1682.2
Chinolunite	$Mg_{6.75}Fe_{2.25}Si_4O_{16}(OH)_{0.5}F_{1.5}$	1.10E-08	-8966.4	-8410.0		1	613.5
Tridymite	SiO_2	1.05E-08	-999.7	-855.9	[4]		2.3
Euxenite	$Y_{0.7}Ca_{0.2}Ce_{0.1}(T_{0.025}O_6)$	1.02E-08	-2671.5	-2506.3		10	136.7
Gersdorffite	$NiAsS$	9.70E-09	N.A.	N.A.	[31]		1189.5
Jarosite	$KFe_3^{2+}(SO_4)_2(OH)_6$	9.57E-09	-3521.7	-3318.7		10	208.5

Continued on next page....

Table 3: Thermodynamic properties of the upper continental crust. – continued from previous page.

Mineral	Formula	ξ_i , mole/g	$\Delta H_{f,i}^\circ$, kJ/mole	$\Delta G_{f,i}^\circ$, kJ/mole	Reference	$\pm \epsilon$, %	$b_{th,i}$, kJ/mole
Humite	$Mg_{3.25}Fe_{1.75}^{2+}(SiO_4)_3 F_{1.5}(OH)_{0.5}$	9.46E-09	-6953.6875	-6512.3		5	504.3
Scheelite	$CaWO_4$	9.28E-09	-1646.2	-1419.6	[4]		139.8
Kornupine	$Mg_{1.1}Fe_{0.2}Al_{5.7}(Si_{13.7}B_{0.3}O_{17.2}(OH)$	9.24E-09	-9172.9	-8624.8		1	173.8
Omphacite	$Ca_{0.6}Na_{0.4}Mg_{0.6}Al_{0.3}Fe_{0.1}Si_{12}O_6$	7.48E-09	-3075.5	-2904.3		1	38.7
Phenakite	Be_2SiO_4	7.31E-09	-2146.2	-2033.3	[4]		34.1
Hisingerite	$Fe_2^{2+}Si_2O_5(OH)_4 \cdot 2(H_2O)$	6.25E-09	-3229.6	-2895.6	[16]		1012.8
Uraninite	UO_2	5.60E-09	-1085.6	-1032.5	[4]		167.6
Malachite	$Cu_2(CO_3)(OH)_2$	5.46E-09	-1052.1	-906.0	[4]		24.3
Strontianite	$SrCO_3$	5.34E-09	-1220.9	-1140.1	[4]		34.9
Brookite	TiO_3	5.27E-09	-942.4	-821.9	[4]		86.5
Perovskite	$CaTiO_3$	5.10E-09	-1662.2	-1575.7	[4]		58.5
Yttrialite	$Y_{1.5}Th_{0.5}Si_2O_7$	4.64E-09	N.A.	N.A.			N.A.
Azurite	$Cu_3(CO_3)_2(OH)_2$	4.38E-09	-1633.3	-1447.5	[4]		350.0
Copper	Cu	3.90E-09	0.0	0.0	[4]		134.0
Pyrochlore	$MgCaNb_2O_6(OH)_{0.75}F_{0.25}$	3.47E-09	-2897.9	-2687.3		10	345.0
Bertrandite	$Be_4Si_2O_7(OH)_2$	3.38E-09	-4586.1	-4300.6		0	72.3
Aemimantite	$Na_2Fe_5^{2+}Ti_5O_{20}$	3.16E-09	-8184.4	-7660.9		10	-164.8
Camotite	$K_2(UO_2)_2(VO_4)_2 \cdot 3H_2O$	2.80E-09	-4907.3	-4585.5	[32]		792.4
Palygorskite	$Mg_6Al_4Si_4O_{10}(OH)_4 \cdot 4(H_2O)$	2.77E-09	-6477.8	-5939.9		1	440.4
Dietzite	$Ca_2(UO_2)_2(CrO_4)$	2.76E-09	-2425.4	-2148.1		10	78.7
Laurite	$Ca(IO_3)_2$	2.76E-09	-1002.5	-839.3	[5]		71.4
Bornite	Cu_5FeS_4	2.65E-09	-334.5	-393.1	[4]		3083.0
Dawsonite	$NaAl(CO_3)(OH)_2$	2.51E-09	-1965.3	-1787.3	[4]		-0.1
Cryolite	Na_3AlF_6	2.36E-09	-3311.3	-3144.7	[4]		327.9
Orpiment	As_2S_3	1.85E-09	-169.1	-168.7	[4]		2641.2
Sulphur	S_8	1.84E-09	0.0	0.0	[4]		4858.2
Zinc	Zn	1.55E-09	0.0	0.0	[4]		339.0
Helvite	$Mn_4Be_3(SiO_4)_3S$	1.45E-09	-5843.9	-5532.4		10	1407.7
Camallite	$KMgCl_3 \cdot 6(H_2O)$	1.45E-09	-2946.7	0.0	[33]		2611.0
Gadolinite	$Y_2Fe^{2+}Be_2(Si_2O_7)_2$	1.41E-09	-5220.0	-4943.3		10	299.7
Xenotime	$YbPO_4$	1.38E-09	-1868.6	-1790.3	[34]		24.2
Nosean	$Na_6Al_6Si_6O_{24} \cdot SO_4$	1.29E-09	-13936.7	-13131.5		5	115.0
Wolframite	$Fe_0.5Mn_{0.5}WO_4$	1.06E-09	-1146.2	-1146.2		1	120.0
Hydrosodalite	$Na_8Al_6Si_6O_{34}(OH)_2$	9.06E-10	-13408.5	-12678.2		5	193.1
Cerussite	$PbCO_3$	8.27E-10	-700.0	-627.5	[4]		20.9
Sibbite	Sb_2S_3	8.10E-10	-175.0	-173.7	[4]		2522.3
Greenockite	CdS	8.01E-10	-162.0	-156.5	[4]		743.9
Chalcoite	Cu_2S	6.83E-10	-79.5	-86.2	[4]		789.1
Smithsonite	$ZnCO_3$	6.36E-10	-813.3	-731.9	[4]		23.3
Blomstrandite	$U_{0.3}Ca_{0.2}Nb_{0.9}T_{0.8}Al_{0.1}Fe_{0.1}^{3+}T_{0.5}O_{16}(OH)$	4.96E-10	-2884.5	-2683.8		10	90.0
Loparite - (Ce)	$Na_{0.6}Ce_{0.22}La_{0.11}Ce_{0.1}T_{0.8}Nb_{0.2}O_3$	4.81E-10	-1430.8	-1343.6		10	181.6
Magnesiocerrite	$MgFe_2^{2+}O_4$	4.40E-10	-1429.4	-1351.0	[4]		40.2
Eudyalite	$Na_4Ca_2Fe_{0.7}^{2+}Mn_{0.3}Zr_5O_{22}(OH)_{1.5}Cl_{1.5}$	4.30E-10	-11859.9	-11062.9		1	335.0
Sirrolite	Zr_2SiO_4	4.02E-10	-2034.8	-1919.2	[4]		20.3
Bischofite	$MgCl_2 \cdot 6(H_2O)$	3.96E-10	-2500.7	-2116.4	[4]		66.0
Tin	Sn	3.87E-10	0.0	0.0	[4]		547.6
Anglesite	$PbSO_4$	3.82E-10	-920.0	-784.5	[4]		62.9
Ramsayite	$Mg_2Ti_2S_2O_9$	3.62E-10	-4360.1	-4103.9	[4]		104.3
Ferrotantalite	$Fe^{2+}Ta_2O_6$	3.07E-10	-2319.3	-2163.9	[4]		174.5
Lead	Pb	3.05E-10	0.0	0.0	[4]		232.2
Chondrodite	$Mg_{3.75}Fe_{1.25}^{2+}(SiO_4)_2 F_{1.5}(OH)_{0.5}$	2.93E-10	-5023.0	-4701.4		5	564.2
Arsenolite	As_2O_3	2.80E-10	-659.8	-579.1	[4]		415.0
Cinnabar	HgS	2.46E-10	-58.2	-50.7	[4]		671.3
Ionsite	FeO	2.38E-10	-272.1	-251.5	[4]		127.3
Britholite	$Ca_2Ce_{0.9}Th_{0.6}La_{0.4}Nd_{0.2}Si_{12.7}P_{0.5}O_{12}(OH)_{0.8}F_{0.2}$	2.18E-10	-7057.3	-6666.9	[35]		734.0
Sodalite	$Na_8Al_6Si_6O_{34}Cl_2$	2.05E-10	-13457.0	-12703.6		10	51.9
Native silver	Ag	1.94E-10	0.0	0.0	[4]		69.7
Axinite- Fe	$Ca_2Fe^{2+}Al_2BO_3Si_4O_{12}(OH)$	1.93E-10	-7640.4	-7180.9		10	427.3
Realgar	As_4S_4	1.40E-10	-140.3	-132.7		0	4272.6

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Table 3: Thermodynamic properties of the upper continental crust. – continued from previous page.

Mineral	Formula	ϵ_r , mol/g	$\Delta H_{f,T}^0$, kJ/mole	$\Delta G_{f,T}^0$, kJ/mole	Reference	$\pm\epsilon$, %	$h_{0,T}$, kJ/mole
Bismuth	Bi	1.30E-10	0.0	0.0	[4]	10	274.8
Bismutite	B ₂ (CO ₃) ₂ O ₂	1.19E-10	-968.7	-888.7			81.1
Rhabdophane	C ₄₀ 75L ₄₀ 25(PO ₄)·H ₂ O	1.03E-10	-1964.9	-1821.9		1	325.0
Bismite	B ₂ O ₃	9.91E-11	-574.3	-493.7	[4]		61.9
Bismuthinite	B ₂ S ₃	9.91E-11	-143.2	-140.6	[4]		2230.8
Baddeleyite	ZrO ₂	9.75E-11	-1101.3	-1043.3	[4]		38.1
Fergusonite	Nd _{0.4} Ce _{0.4} S _{1.0} Y _{0.1} NbO ₄	8.08E-11	-2808.3	-2631.2	[4]	10	-717.4
Cobaltite	CoAsS	5.06E-11	-163.1	N.A.		1	N.A.
Smalite	CoAs ₂	5.06E-11	-61.5	N.A.	[5]		N.A.
Argentite	Ag ₂ S	4.99E-11	-29.4	-39.4	[4]		707.3
Cancrinite	N ₆₆ C ₂ Al ₆ Si ₁₆ O ₂₄ (CO ₃) ₂	4.20E-11	-14980.9	-14136.3		10	101.8
Moissanite	SiC	3.51E-11	-62.8	-60.3	[4]		1204.1
Uranium-Thorite	ThSiO ₄	3.18E-11	-2160.5	-2048.8	[4]	5	27.8
Powellite	CaMoO ₄	3.05E-11	-1542.4	-1434.7	[4]		27.6
Chevkinitite	Ce _{1.7} La _{1.4} Ce _{0.8} Th _{0.1} Fe _{2.8} ²⁺ Mg _{0.5} Ti _{2.5} Fe _{0.5} ³⁺ Si ₄ O ₂₂	2.76E-11	-10499.8	-9894.5		10	1006.2
Acanthite	Ag ₂ S	2.74E-11	-32.4	-40.3	[4]		706.4
Lavenite	Ni _{1.1} Cu _{0.9} Mn _{0.2} Fe _{0.5} ²⁺ Zn _{0.8} Ti _{0.1} Nb _{0.1} (S ₂ O ₇) _{0.6} (OH) _{0.3} F _{0.1}	2.59E-11	-4191.1	-3925.1		10	604.8
Pyrrhotite	Ag ₃ As ₃	2.38E-11	-131.5	-142.2		5	2325.9
Linnaeite	Co ₃ S ₄	1.69E-11	-307.3	-323.6	[4]		3032.2
Thorianite	ThO ₂	1.56E-11	-1227.2	-1169.6	[4]		48.8
Troilite	FeS	1.19E-11	-100.5	-99.9	[4]		884.2
Microcline	Nd _{0.4} Ce _{1.6} Ti _{0.2} O _{6.6} (OH) _{0.3} F _{0.1}	8.71E-12	-3208.3	-3004.3	[4]	10	315.1
Delorenzite	Y _{0.7} Co _{0.2} Ce _{0.12} (Th _{0.07}) ₂ (Nb _{0.2}) ₂ (Ti _{0.1}) _{0.5} (OH) _{0.5}	8.33E-12	-2721.2	-2549.9		10	54.6
Stephanite	Ag ₅ As ₄	7.72E-12	-166.1	-184.5		5	3030.3
Naegite	ZrSiO ₄	6.98E-12	-2034.8	-1919.2	[4]		20.3
Gold	Au	6.47E-12	0.0	0.0	[4]		51.5
Lamprophyllite	Ni ₂ SrBaTi ₃ Si ₄ O ₁₆ (OH)F	5.61E-12	-8401.2	-7865.3		10	892.0
Chlorargente	AgCl	5.47E-12	-127.2	-109.9	[4]		22.0
Periclase	MgO	3.77E-12	-602.2	-569.5	[4]		62.1
Chrysocholla	Cu ₂ Si ₂ O ₆ (H ₂ O) ₄	3.54E-12	-3279.4	-2964.6		10	-23.9
Freibergite	Ag _{7.2} Cu _{3.6} Fe _{1.2} Sb ₃ As _{1.3}	3.52E-12	-703.2	-727.5		5	10786.0
Metacinnabar	HgS	3.17E-12	-53.6	-47.7	[4]		674.3
Vivianite	Fe ₃ (PO ₄) ₂ (H ₂ O) ₈	2.59E-12	-4608.4	-4428.2		10	457.4
Cooperite	Pb _{0.6} Pb _{0.3} Ni _{0.1} S	2.11E-12	-79.8	-73.8		1	688.3
Misericite	KC _{0.2} Ce _{3.8} O ₂₂ (OH) _{1.5} F _{0.5}	2.00E-12	-11738.2	-11035.1	[32]	10	1138.1
Torbernite	Cu ₂ (UO ₂) ₂ (PO ₄) ₂ ·8(H ₂ O)	1.81E-12	-4455.9	-4129.8		0	-35.2
Weinschenkite	YPO ₄	1.68E-12	-1987.7	-1871.1	[4]		151.6
Wulfenite	PbMoO ₄	1.66E-12	-1112.9	-952.8		0	1284.7
Loellingite	FeAs ₂	1.30E-12	-85.7	-80.2	[4]	0	9965.1
Tennantite	Cu ₁₀ Fe ₂ As ₄ S ₁₃	1.24E-12	-1968.6	-1999.6		0	60.0
Tellurite	TeO ₂	1.14E-12	-322.8	-270.3	[4]		N.A.
Sylvanite	Ag _{0.75} Ag _{0.25} Te ₂	7.62E-13	N.A.	N.A.		10	958.5
Nordite	Ni _{2.8} Mn _{0.2} Sr _{0.5} Ca _{0.5} La _{0.33} Ce _{0.6} Zn _{0.6} Mg _{0.4} S ₁₆ O ₁₇	7.20E-13	-8020.8	-7532.2		0	686.8
Calaverite	AuTe ₂	5.71E-13	-19.0	-17.4		5	4817.9
Saunsonite	Ag ₄ MnS ₆ S ₆	5.29E-13	-444.9	-463.5		0	9797.1
Tetraedrite	Cu ₁₀ Fe ₂ S ₁₂ S ₁₃	3.47E-13	-1909.5	-1939.7		0	50.5
Thortveitite	Sr _{1.5} Y _{0.5} S ₁₂ O ₇	2.71E-13	-3740.2	-100.6		1	1709.0
Tetradymite	Bi ₂ Te ₃	2.27E-13	-100.2	-100.6		10	1441.1
Rinkite	Ni _{0.2} Ce _{1.5} Y _{0.5} Ti _{0.4} Nb _{0.5} Zr _{0.1} (S ₂ O ₇) ₂ O _{1.5} F _{0.5}	2.25E-13	-9415.1	-8808.5	[4]		127.3
Alunite	KAl ₃ (SO ₄) ₂ (OH) ₆	2.20E-13	-5173.2	-4652.2			N.A.
Osmium	O ₃₀ 75Ir _{0.25}	1.57E-13	N.A.	N.A.			N.A.
Iridium	Ir _{0.5} O _{0.3} As _{0.2}	1.50E-13	N.A.	N.A.			N.A.
Dumortierite	Al _{6.9} (BO ₃) ₅ (SiO ₄) ₃ O _{2.5} (OH) _{0.5}	1.33E-13	-9109.0	-8568.0	[36]		108.9
Polycrase (Y)	Y _{0.5} Ce _{0.1} Ce _{0.1} U _{0.1} Th _{0.1} Ti _{1.2} Nb _{0.6} Ta _{0.2} O ₆	2.46E-14	-2847.7	-2681.3		10	125.4
I-Platinum	Pt	1.54E-14	0.0	0.0	[4]		146.5
Polixene/ Tetraferro-platinum	PtFe	1.20E-14	N.A.	N.A.			N.A.
Boulangierite	Pb ₅ S ₄ S ₁₁	2.12E-15	-1034.5	-1023.7		5	8565.5
Wohlerite	Ni ₂ Ce ₂ Zr _{0.6} Nb _{0.4} Si ₂ O _{8.4} (OH) _{0.3} F _{0.3}	1.27E-15	-4439.7	-4170.0		10	466.6

End of the table