FORMATION AND STABILITY OF SUBSTITUTED PYROMORPHITE: A MOLECULAR MODELING STUDY

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ABSTRACT

Soils contaminated with lead pose significant risk to human as well as terrestrial and aquatic ecosystems. Theoretical phase relationships and field observations suggest that the interaction of lead and phosphorus to form pyromorphites $Pb_5(PO_4)_3X$ ($X = OH^-$, Br^-, Cl^-, or F^-) is an important buffer mechanism controlling the migration and fixation of lead in the environment. We report a molecular modeling approach to investigate the formation and stability of the substituted pyromorphites, which involved evaluating the lattice energy of the minerals using *ab initio* quantum mechanics. The lattice energy values are used in a Born-Haber thermodynamic cycle to calculate the heat of formation of the minerals. The Gibbs free energy of the substituted pyromorphites is then calculated from the change in entropy and heat of formation. The systems investigated in this study include partial and total substitution of Pb^{2+} by Cd^{2+} and Zn^{2+} cations in chloropyromorphite ($Pb_5(PO_4)_3Cl$). Results indicate the unstable nature of the substituted Pb pyromorphite. The stability of the substituted minerals is found in the order Pb-pyromorphite > Cd-pyromorphite > Zn-pyromorphite.

Key words: pyromorphite, substitution, stability, formation, molecular modeling

INTRODUCTION

Heavy metal contamination of soils is common at many hazardous waste sites. Lead (Pb), cadmium (Cd), zinc (Zn), chromium (Cr), and mercury (Hg) are commonly observed contaminants from activities such as vehicle emission, mining, smelting, and agricultural/industrial chemical applications (Chen and Hong, 1995; EPA, 1992; Lambert et al., 1997; McClean et al., 1992). The adverse impact of heavy metal contaminants on environmental quality and on human health is also known. The current study will focus on Pb as the element of concern in the Tri-State mining region (southeast Kansas, southwest Missouri, and northeast Oklahoma), where Pb and Zn sulfide ores have been mined since 1870 to 1970. The remediation of heavy metals in the soil matrix is difficult because of their retention. In general, the preferred remediation option available is soil removal (EPA, 1996). Other options for excavated materials include solidification, vitrification, washing, and leaching (EPA, 1992; Pierzynski et al., 1994). Recently, the idea of amending Pb-contaminated soils with phosphorus (P) as an *in situ* remediation option has been proposed as an alternative to soil removal (EPA, 1996). It has been recognized for some time that Pb phosphates are very stable under environmental conditions (Nriagu, 1974). Lead reacts with soluble P to form various pyromorphites [$Pb_5(PO_4)_3X$, where $X = OH^-$, Br^-, Cl^-, or F^-] that are very insoluble. The formation of Pb-pyromorphites is critically determined by the availability of phosphorous in soils. For heavy metal phosphate formation, free phosphate ions ($H_nPO_4^{-3}$) must be available in the soil, so more soluble forms of P are useful for Pb-pyromorphite formation (Cotter-Howells et al., 1996).

The most likely source of soluble P would be common fertilizer materials. Early work identified pyromorphite with a scanning electron microscope (SEM) in Pb-contaminated soils and suggested that the occurrence of Pb in this form limited blood Pb-concentrations in children living in the area (Cotter-Howells and Thornton, 1991). Later work suggested that pyromorphite was a natural weathering product in Pb contaminated soils (Cotter-Howells et al., 1994; Klein et al., 1993). Suggestions of using P to immobilize Pb in aqueous solutions or in soils soon followed (Cotter-Howells and Caporn, 1996; Hettiarachchi et al., 2000; Ma et al., 1993; Ruby et al., 1994). Because zinc and cadmium often occur simultaneously with Pb in contaminated soils, the potential participation of the Zn^{2+} and Cd^{2+} in the formation of lead phosphates is of interest.

Pyromorphites belong to the apatite group of minerals. The most common member of the apatite family is fluorapatite ($Ca_5(PO_4)_3F$). The structural characteristics of fluorapatite is such that various ions belonging to groups I, II, and III, as well as Pb^{2+}, Zn^{2+}, Cd^{2+}, etc., can substitute for Ca^{2+} while SO_4^{2-}, CO_3^{2-}, CrO_4^{2-}, etc., can be substituted for PO_4^{3-} (Botto, 1997). Baravelli et al. (1984) have also reported the substitution of many bivalent metal cations such as Mg^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, and Ni^{2+} for Ca^{2+} in hydroxyapatite ($Ca_5(PO_4)_3OH$). They found that these substitutions resulted in a reduction in the degree of the crystallinity of the apatite phase. There have also been a few studies that target possible substitutions occuring in the naturally existing pyromorphites (Botto et al., 1997; Cotter- Howells et al., 1994). The substitution of Pb^{2+} by Ca^{2+} and Ba^{2+} ions, and Cl^- by OH^- has been detected. These studies are experimental and are aimed at identifying and characterizing the substituted pyromorphites. The thermochemical data (e.g., heat of formation, solubility product, etc.) that are necessary to determine the formation and stability of these substituted minerals were not reported. The important issue is whether the partial or total substitution in Pb pyromorphite by other metal ions such as Cd^{2+}, Zn^{2+} ions, etc., that frequently occur simultaneously with Pb^{2+}, is favorable or not. Hence we have chosen to thermodynamically evaluate the formation and stability of these partial or total substituted chloropyromorphite minerals. We know of no previous theoretical study targeting this issue. In the subsequent sections, we report a molecular modeling approach to predict the formation and stability of substituted chloropyromorphites formed by partial or total substitution of Pb^{2+} by the competing cations Cd^{2+} and Zn^{2+}. In this approach, lattice energy values evaluated by *ab initio* quantum mechanics are used in a Born-Haber thermodynamic cycle to calculate the heat of formation of the substituted chloropyromorphites. This is followed by predicting the entropy changes based on the entropy of the minerals and their constituent elements. The solubility product of the minerals is then calculated from the Gibbs free energy, which is evaluated from the heat of formation and change in entropy.
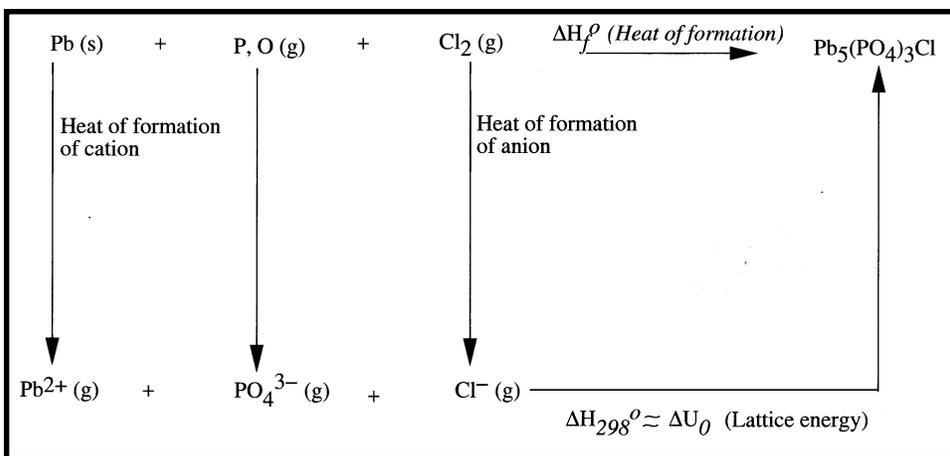
Figure 1. Born-Haber cycle to predict the formation of Pb-pyromorphite.

2.1 THEORY

The gibbs free energy of an ionic crystal is calculated using the equation

$$\Delta G^{o}_{f} = \Delta H^{o}_{f} - T\Delta S^{o}_{f} \tag{1}$$

where ΔG^{o}_{f}, ΔH^{o}_{f}, and $T\Delta S^{o}_{f}$ are the standard Gibbs free energy, heat of formation, and entropy change, respectively, of the crystal. The estimation of Gibbs free energy (ΔG^{o}_{f}) for ionic compounds usually involves separate estimation of the contributing entropy ($T\Delta S^{o}_{f}$) and heat of formation (ΔH^{o}_{f}) terms. The estimation of entropy change (ΔS^{o}_{f}) of an ionic crystal require knowledge of the entropy (S^{o}_{f}) of the ionic compound and its constituent elements in their standard states. Latimer (1952) has provided means of assessing the value of S^{o}_{f} for ionic compounds by tabulating the average contributions made by various ions to the total entropy of the solid. The entropy values of the constituent elements have also been listed (Dasent, 1970). The heat of formation (ΔH^{o}_{f}) of the Pb pyromorphite crystal is evaluated by setting up a Born-Haber thermodynamic cycle as shown in Figure 1. As seen from Figure 1, the heat of formation of the crystal depends on the heat of formation of the individual cations and anions in the gas phase, and the lattice enthalpy ΔH_{298}. The heat of formation of gaseous cation is, in the case of monoatomic species, the sum of heat of atomization and the heat of ionization. The appropriate experimental data (heats of sublimation of metals and ionization potentials) are available in most cases. In the case of monoatomic anions, the heat of formation is similarly the sum of heat of atomization and an electron affinity, and again the experimental data are available for common species, such as the halide anion. The lattice enthalpy ΔH_{298} is given as

$$\Delta H_{298} = \Delta U_{o} + \int_{0}^{298} \left[c_{p}(crystal) - c_{p}(ion) \right] dT, \tag{2}$$

where ΔU_o is the lattice energy at 0 K, c_p is constant pressure heat capacity, and T is the absolute temperature. For calculations, it is often assumed that the lattice energy does not alter much with temperature (Dasent, 1970) and hence $\Delta H_{298} \approx \Delta U_o$. Lattice energy is defined as the energy liberated when a mole of the requisite free gaseous ions comes together from infinite inter ionic separation to form a crystal (Swaddle, 1990). The simplest empirical expressions of lattice energies are obtained by regarding the crystal as an assembly of spherical ions (i.e., by adopting a pure ionic model) and by evaluating (a) the energy of the attractive coulombic forces between the oppositely charged ions, and (b) the repulsive forces resulting from the interpenetration of the spherical charged clouds of the ions. Kapustinski (1956) has developed expressions for the lattice energy for use in cases where experimental data are lacking. These equations are only applicable to sixfold coordina-tion of NaCl-type crystal. There is no satisfactory experimental method for measuring lattice energies directly. Hence we use *ab initio* quantum mechanics to predict ΔU_o for the substituted pyromorphite. Knowing the heat of formation of individual ions in gas phase and the lattice energy, one should be able to calculate the heat of formation (ΔH^o_f) of the crystal. In equation (1), the enthalpy changes in all cases are much larger than the entropy terms (Swaddle, 1990), and the enthalpy contribution dominates ΔG^o_f. Normally, the value of $T\Delta S^o_f$ is negative in all cases for the reaction described in the Born-Haber cycle.

2.2 MOLECULAR MODELING APPROACH

Atomistic computer modeling techniques play an important role in studying both structural and dynamical properties, and the reactivity of solids (Catlow et al., 1997). *Ab initio* quantum mechan-ics (QM) techniques are the most accurate molecular modeling methods. Requiring only the atomic number of an element, they relate molecular and solid properties to the interactions of electrons. All QM methods work by approximating a solution to the Schrodinger equation. The disadvantage of QM methods has been that even approximate solutions for simple systems can be complex. Among quantum mechanical methods, the choice is between first-principle and semiempirical methods. First-principle methods include Density Functional Theory (DFT) and Hartree-Fock (HF). These methods are computationally expensive (depending on the system under investigation), and can be used to predict highly accurate molecular and solid state properties. While the semi empirical methods are computationally less demanding, they have the disadvantage of being applicable to only molecular systems. In recent years, however, improvement in numerical algorithms and com-puter hardware has made first-principles calculations on practical systems more feasible. At the same time, new methods offering novel approximations have enabled QM methods to be applied and extended to solid state systems. One such approach, called as Fast Structure (from Molecular Simulations Inc.), can be used to predict the lattice energies of the minerals. Fast Structure is an *ab initio* software package based on a DFT approach specifically designed to determine the structure
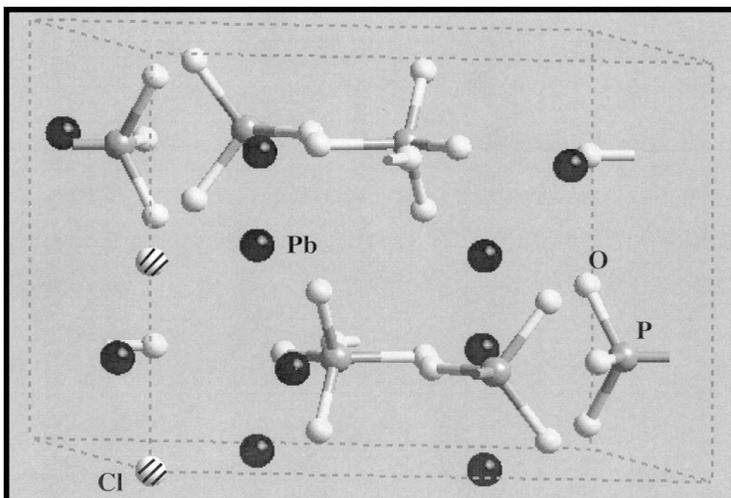
Figure 2. Schematic of a unit cell of the Pb-pyromorphite $Pb_{10}(PO_4)_6Cl_2$ crystal.

of molecules, solids, and surfaces by calculating the energy and force acting on the nuclei, and determining the nuclear locations corresponding to the energy minimum. Fast structure achieves its speed via algorithmic improvements (e.g., by the use of the so called Harris function) (Harris, 1985). The base set in this approach (from Molecular Simulations Inc.) is defined by the core choice (FULL, RELAXED, or FROZEN), orbital choice (MINIMAL, STANDARD, or EN-HANCED), the density basis choice (MINIMAL, STANDARD, or ENHANCED), and the cutoff radius. For the present investigation, the FULL core basis option is used. This treatment considers the core electrons to be the same as the valence electrons. The orbital basis uses the STANDARD treatment, where for each valence electron an additional basis function is added to the MINIMAL orbital basis choice. The MINIMAL choice for basis density results in the use of one basis function for all valence electrons. A cutoff value of 0.5 nm is used in present calculations. The cutoff radius is used by the Fast Structure approach for reconstructing the atomic density and orbitals. This helps in avoiding the overlap between the orbitals centered on different atoms. The lattice energy reported by Fast Structure is calculated as the difference between the total energy of the crystal per formula unit (computed for the optimized equilibrium structure) and the energies of the isolate atoms. The results of Fast Structure are of comparable accuracy as compared to other available approaches, such as CASTEP, ESOCS (from Molecular Simulations Inc.), etc. It can also be used to perform dynamical calculations on an ensemble at a given, constant energy or temperature.

The crystal data of pyromorphite (Dai, 1989) is used to build a crystal using the software package Cerius2 (from Molecular Simulations Inc.). The crystal structure of Pb pyromorphite is shown in Figure 2. The substituted pyromorphites $M_xPb_{5-x}(PO_4)_3Cl$ in this study were formed by substituting x number of Cd^{2+} and Zn^{2+} ions as M for Pb^{2+}.

3. RESULTS AND DISCUSSION

3.1 Formation of Substituted Cl-Pyromorphites

The lattice energy (or binding energy) values of the substituted pyromorphite (for x=1,3,5), calculated using *ab initio* quantum mechanics, are shown in Table 1. Based on the lattice energy values, it can be seen that the order of decreasingly negative lattice energy for Cd^{2+} substitutions for Pb^{2+} in Pb pyromorphite is $CdPb_4(PO_4)_3Cl < Cd_3Pb_2(PO_4)_3Cl < Cd_5(PO_4)_3Cl$. A similar lattice energy trend is followed by Zn^{2+} for its partial and total substitution of Pb^{2+} ions, giving $ZnPb_4(PO_4)_3Cl < Zn_3Pb_2(PO_4)_3Cl < Zn_5(PO_4)_3Cl$. Comparing the individual ion lattice energies for various substitutions, it can been seen that the Cd^{2+} ion substitution has lower lattice energy values as compared to Zn^{2+} for their partial and total substitution of Pb^{2+} ions in the pyromorphite. It can also be seen that the $Pb_5(PO_4)_3Cl$ has the lowest lattice energy value as compared to all other substituted minerals, and it increases as the number of substitutions for the Pb^{2+} increases. We could roughly define a qualitative stability based on the lattice energy and conclude that Pb pyromorphite is the most stable phase, followed by Cd and Zn substituted pyromorphite.

In the previous section, we discussed that the heat of formation of a crystal could be determined by designing a Born-Haber cycle (see Figure 1). By knowing the heat of formation of the individual constituent ions in the gas phase and the lattice energy, we can calculate the heat of formation of the crystal. We first take Pb pyromorphite as a test case to compare the experimental and theoretical predictions of ΔG°_f. A Born-Haber cycle is set up to evaluate the heat of formation of the Pb pyromorphite. The lattice enthalpy of Pb pyromorphite is calculated for the following equation:

$$5Pb^{2+}(g) + 3(PO_4^{3-})(g) + Cl^-(g) \rightarrow Pb_5(PO_4)_3Cl(s). \tag{3}$$
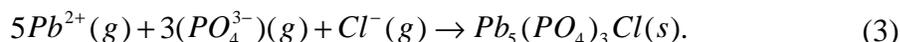
The thermochemical data for various ionic species and compounds is summarized in Table 2. The heat of formation of the phosphate ion $\left(PO_4^{3-} \right)$ in the gas phase is not known, though the heat of formation in the liquid phase is known (Swaddle, 1990). Because the formation of PO_4^{3-} in gas

Table 1. Lattice energy of substituted pyromorphites

Mineral	Lattice energy (kJ/mol)
$Pb_5(PO_4)_3Cl$	-13163.82
$CdPb_4(PO_4)_3Cl$	-12980.19
$ZnPb_4(PO_4)_3Cl$	-12875.79
$Cd_3Pb_2(PO_4)_3Cl$	-12602.45
$Zn_3Pb_2(PO_4)_3Cl$	-12281.96
$Cd_5(PO_4)_3Cl$	-12240.71
$Zn_5(PO_4)_3Cl$	-11806.12

phase has not been reported in literature, the heat of formation of $H_2PO_4^-$ will be used to approximate the ΔH^o_f of the phosphate ion. This assumption is justified by the fact that incorporation of $H_2PO_4^-$ in the phosphate ion sites has been previously reported (Botto et al., 1997) in the fluorapatite structure. The gas-phase acidity of phosphoric acid (H_3PO_4) to form $H_2PO_4^-$ (Blades et al., 1996; Morris et al., 1997) is given by

$$H_3PO_4(g) \rightarrow H^+(g) + H_2PO_4^-(g) \qquad \Delta H^o_r = 1383 \ kJ/mol, \qquad (4)$$

where ΔH^o_r is the heat of reaction. The heat of formation of $H_2PO_4^-$ in the gas phase can be evaluated knowing the heat of formation values of H^+ and H_3PO_4 in the gas phase from equation (4). This value was calculated to be -742.38 kJ/mol. Using the Born-Haber cycle and knowing the heat of formation of Pb^{2+}, $H_2PO_4^-$ and Cl⁻ ions in the gas phase, the heat of formation (ΔH^o_f) of Pb pyromorphite is calculated as -3754.80 kJ/mol. The entropy change (ΔS^o_f) is calculated based on the knowledge of total entropy of the Pb pyromorphite crystal through the average contributions made by the individual ions in the solid phase and also the contributions to the entropy made by the reacting ions in their standard states (Dasent, 1970). The total calculated entropy S^o_f values for the

Table 2. Thermochemical data for ionic species in gaseous/aqueous phase at 298 K

Compound	ΔH^o_f (kJ/mol)	ΔS^o_f (kJ/mol)	ΔG^o_f (kJ/mol)
Pb^{2+}(l)[a]	-	-	-24.39
Pb^{2+}(g)[b]	2373	-	-
Cd^{2+}(l)[b]	-	-	-77.73
Cd^{2+}(g)[b]	2623.85	-	
Zn^{2+}(l)[b]	-	-	-147.19
Zn^{2+}(g)[b]	2781.94	-	-
H^+(g)[c]	1530	-	-
Cl⁻(l)[a]	-	-	-131.25
Cl⁻(g)[c]	-233	-	-
PO_4^{3-}(l)[a]	-	-	-1018.9
H_3PO_4(g)[d]	-595.38	-	-
$H_2PO_4^-$(l)[c]	-	90.4	-
$H_2PO_4^-$(g)[e]	-742.36	-	-

[a] Nriagu, 1974
[b] Rossini *et al.*, 1952
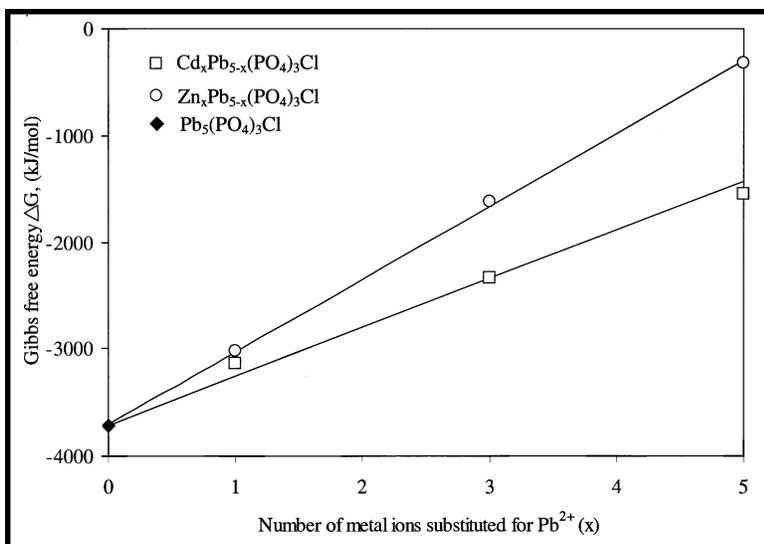[c] Swaddle, 1990
[d] Karpet'yants, 1970
[e] This Work

Figure 3. Gibbs free energy (ΔG^o_f) values for the partial and total substitutions of Cd^{2+} and Zn^{2+} cations for Pb^{2+} in Pb-pyromorphite.

reactants (individual ions) and the product (solid) are 702 J/mol K and 572 J/mol K, respectively. Thus, we can see the expected decrease in entropy when the solid is formed. The contribution by the $-T\Delta S^o_f$ term is only 38.74 kJ/mol, which is very small as compared to ΔH^o_f. The Gibbs free energy (ΔG^o_f) is then calculated using equation (1). The predicted value for $Pb_5(PO_4)_3Cl$ from the molecular modeling approach is -3716.06 kJ/mol, which is close to the reported experimental value of -3791.54 kJ/mol (Nriagu, 1974). The ΔH^o_f and ΔG^o_f values of other substituted pyromorphites are calculated in the same way, and are tabulated in Table 3. It can be seen that the order of decreasingly negative Gibbs free energy for the Cd^{2+} substitution for Pb^{2+} in pyromorphite is $CdPb_4(PO_4)_3Cl < Cd_3Pb_2(PO_4)_3Cl < Cd_5(PO_4)_3Cl$. The order of ΔG^o_f values for Zn^{2+} substitution in pyromorphite also follows the same trend as Cd^{2+}. The Gibbs free energy value increases

**Table 3.** Predicted thermodynamic data for the substitued pyromorphites at 298 K

Mineral	ΔH^o_f (kJ/mol)	$-T\Delta S^o_f$ (kJ/mol)	ΔG^o_f (kJ/mol)
$Pb_5(PO_4)_3Cl$	-3754.80	38.74	-3716.06*
$CdPb_4(PO_4)_3Cl$	-3173.56	39.54	-3134.02
$ZnPb_4(PO_4)_3Cl$	-3060.30	38.81	-3021.49
$Cd_3Pb_2(PO_4)_3Cl$	-2369.60	38.35	-2330.75
$Zn_3Pb_2(PO_4)_3Cl$	-1648.66	36.38	-1612.28
$Cd_5(PO_4)_3Cl$	-1581.48	37.16	-1544.32
$Zn_5(PO_4)_3Cl$	-356.43	33.88	-322.55

*Experimental value -3791.54 kJ/mol (Nriagu, 1974).

with the number of Pb^{2+} ions substituted. The Gibbs free energy values of the substituted Cd and Zn pyromorphites are plotted in Figure 3 along with that of Pb pyromorphite. It can be seen that the Pb pyromorphite crystal has the lowest ΔG^o_f value. Interestingly, the trends observed for ΔG^o_f values for the substituted pyromorphites are similar to those for lattice energy.

4. STABILITY OF SUBSTITUTED PYROMORPHITES

The stability of a compound is determined by its solubility product, K_{sp}. The solubility product for Pb-pyromorphite can be evaluated using the following equations:

$$Pb_5(PO_4)Cl(s) \rightarrow 5Pb^{2+}(l) + 3PO_4^{3-}(l) + Cl^-(l). \tag{5}$$
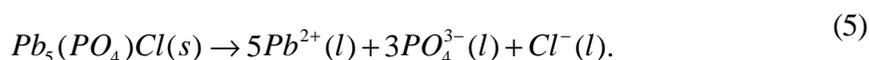
$$\Delta G^0_{reaction} = \Delta G^o_{product} - \Delta G^o_{reactant} = -2.303 \, RT \, logK_{sp}, \tag{6}$$

where R is the universal gas constant. The theoretically predicted value of $logK_{sp}$ for Cl-pyromorphite, using data from Tables 2 and 3, is -72.12, while the experimental $logK_{sp}$ is -84.47. Solubility products for the Cd- and Zn- substituted pyromorphites are listed in Table 4. It can be seen that these are highly soluble (even higher than PbO, which has a $logK_{sp}$ of 12.9). It can be concluded that the partial and total substitution of Cd^{2+} and Zn^{2+} ions for Pb^{2+} may affect the cystallinity of the original pyromorphite due to the different sizes of the ions being substituted for Pb^{2+}. This kind of instability has also been observed previously for substitutions in hydroxyapatite (Baravelli et al., 1984). Thus, the partial and total substitution of the other metal cations for Pb^{2+} affects morphology and stability of the substituted pyromorphites. Table 5 shows some lead, cadmium, and zinc phosphates that are found in soil. It can be seen that Pb-pyromorphite is highly stable and hence is

Table 4. Predicted solubility product of the substutued pyromorphites at 298 K

Mineral	$logK_{sp}$
$Pb_5(PO_4)_3Cl$	-71.12*
$CdPb_4(PO_4)_3Cl$	40.01
$ZnPb_4(PO_4)_3Cl$	72.04
$Cd_3Pb_2(PO_4)_3Cl$	199.56
$Zn_3Pb_2(PO_4)_3Cl$	362.07
$Cd_5(PO_4)_3Cl$	356.21
$Zn_5(PO_4)_3Cl$	631.21

*Experimental value -84.47 kJ/mol (Nriagu, 1974).

Table 5. Solubility products of some lead, zinc, and cadmium phosphate minerals at 298 K

Mineral	$logK_{sp}$
$Pb_5(PO_4)_3Cl$	-84.4
$Pb_5(PO_4)_3OH$	-82.3
$Pb_5(PO_4)_3F$	-71.6
$Zn_3(PO_4)_2.4H_2O$	-35.3
$Zn_2(PO_4)_3OH$	-26.6
$Zn_4(PO_4)_2(OH)_2.3H_2O$	-52.8
$Zn_5(PO_4)_3OH$	-63.1
$Cd_3(PO_4)_2$	-38.1

*Data from Nriagu, 1974 and 1984.

thought to control the lead activities in the natural system. In the case of zinc, it can be assumed that hopeite ($Zn_3(PO_4)_2 \cdot 4H_2O$) may regulate zinc in the ecosystem (Nriagu, 1974). Cadmium phosphates are very rare in nature; this could be attributed to the low cadmium activity in soils (Barak et al., 1993).

5. CONCLUSIONS

In this work the partial and total substitution of Pb^{2+} by Cd^{2+} and Zn^{2+} ions in Cl-pyromorphite are studied by *ab initio* quantum mechanics. Results show that ΔH^o_f and ΔG^o_f values of the substituted Cl-pyromorphites show the same trend as seen in the lattice energy values. The calculated solubility products of the substituted Cl-pyromorphites indicate the highly unstable nature of the substituted minerals. The stability of the substituted minerals is found in the order Pb-pyromorphite $\gg$ Cd- pyromorphite $>$ Zn-pyromorphite for all substitutions. Both partial and total substitutions of Pb^{2+} by Cd^{2+} and Zn^{2+} seem to be unfavorable; this may be due to the effect of substitution on the crystallinity and morphology of the pyromorphite structure. The molecular modeling approach can serve as an important tool for predicting the formation and stability of complex crystals whose experimental data are not available.

The nomenclature is presented in Table 6.

6. ACKOWLEDGEMENTS

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Table 6. Nomenclature

ΔU_o	Lattice or binding energy at 0 K	kJ/mol
c_p	Constant pressure heat capacity	kJ/mol K
T	Absolute temperature	K
R	Universal gas constant	kJ/mol K
ΔG^o_f	Standard Gibbs free energy	kJ/mol
ΔH^o_f	Standard heat of formation	kJ/mol
ΔS^o_f	Standard entropy	J/mol K

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