Preparation and FT–IR Characterization of Metal Phytate Compounds

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ABSTRACT

Phytic acid (inositol hexaphosphoric acid, IP6) has long been recognized as the predominant organic P form in soil and animal manure. Whereas many studies have investigated the wet chemistry of IP6, there is little information on the characterization of solid metal IP6 compounds. This information is essential for further understanding and assessing the chemical behavior of IP6 in diverse soil–plant–water ecosystems. As the first step in full characterization, we synthesized eight metal phytate compounds and investigated their structural features using Fourier transform infrared spectroscopy (FT–IR). The absorption features from 900 to 1200 cm⁻¹ in FT–IR could be used to identify these phytates as: (i) light divalent metal (Ca and Mg) compounds with a sharp band and a broad band, (ii) heavy divalent metal (Cu and Mn) compounds with splitting broad bands, and (iii) trivalent metal (Al and Fe) compounds with a broad band and a shoulder band. Three different types of chemical structures of metal–phytate compounds were presented based on the FT–IR information. We further demonstrated that metal orthophosphates possessed different FT–IR spectral characteristics from their IP6 counterparts. The unique spectral features of metal phytates from 1000 to 700 cm⁻¹ could be used to distinguish phytate compounds from metal phosphate compounds. Thus, FT–IR analysis after fine tuning could provide an analytical tool to investigate the basic metal phytate chemistry in molecular levels, such as the competitive interactions between phosphate and phytate with a specific metal ion, and the conversion (or hydrolysis) of metal phytate to metal phosphate under various conditions.

Phytic acid (inositol hexaphosphoric acid, IP6) has been identified as an important organic P form in soil, animal manure, and other environmental samples (Anderson et al., 1974; Caldwell and Black, 1958; Celi et al., 2003; He et al., 2004a, 2004b, 2006a; Turner et al., 2002). It contains a 6-C ring with 1 H and 1 phosphate attached to each C. Each of the 6 phosphate groups is attached in an ester linkage and retains two replaceable hydrogens. These two nonester hydroxyl groups should impart some inorganic P-like (orthophosphate bond) properties to IP6, leading to interactions of IP6 with various metal ions in the environment to form various soluble or insoluble compounds (phytate salts). Dao (2003, 2004a, 2004b) investigated the effects of cations (Na, Ca, Al, and Fe) and several organic ligands on phosphatase hydrolysis of IP6. His work showed that Al and Fe inhibited phosphatase hydrolysis (dephosphorylation) by precipitating IP6. Dependent on the metal/ligand ratios, this inhibition was relieved or totally removed by addition of organic ligands (Dao, 2004a), indicating that bioavailability of IP6-P is regulated not only by pH-controlled IP6-hydrolysis enzymatic activity but also the associated counterions and organic ligands in the environment. Reducing conditions (He et al., 2006b) and competitive adsorption or formation of aqueous ternary dissolved organic matter–Fe (or Al)–PO₄ complexes, a mechanism of increasing P dissolution in soils (Hutchison and Hesterberg, 2004), can also affect the phytate solubility in the environment.

Ognalaga et al. (1994) found that glucose-1-phosphate and IP6 are absorbed on surface hydroxyls of goethite (αFeOOH) through their phosphate groups. Celi et al. (1999, 2001) reported that the adsorption of IP6 on αFeOOH involves the phosphate group, whereas the organic moiety of IP6 affects the process only in terms of conformational hindrance. Furthermore, the adsorption increased with Ca ions but decreased in the presence of K with increasing pH (Nash et al., 1998). Seaman et al. (2003) reported that soluble IP6 can precipitate with native polyvalent cations (such as Ca and Mg) and further coprecipitate or exchange with heavy metals in heavy metal–contaminated soils or sediments. These studies provide valuable information on the interactions of IP6 with metal ions; however, relatively few studies have characterized the metal IP6 compounds themselves (Evans and Pierce, 1982; Graf, 1983; Kaufman and Kleinberg, 1971). Because of the lack of such basic information, it is very difficult to formulate hypotheses without speculation to account for the behaviors of IP6 in the environment. Due partly to the lack of model compounds for reference, identification of metal IP6 species in animal manures and in soils by advanced solid state spectroscopic analysis, such as X-ray absorption near edge structure (XANES) spectroscopy (Peak et al., 2002) and solid state ³¹P nuclear magnetic resonance (NMR) spectroscopy (Hunger et al., 2004), has not been accomplished. Information on metal IP6 species and their dynamics is essential to completely and comprehensively understanding the chemical behaviors of both metals and organic P in various ecosystems.

The objectives of this study were to (i) synthesize eight metal IP6 compounds and (ii) initiate their characterization to increase our knowledge of metal IP6...
compound chemistry and to provide spectral data for more accurately identifying these compounds in environmental samples.

MATERIALS AND METHODS

Preparation of Metal IP6 Compounds

Phytic acid dodecasodium salt (Na12IP6, C6H6O24P6Na12, minimum 90% purity) and metal chlorides were used to prepare metal IP6 compounds. For the preparation of IP6 compounds of Ca, Mg, Cu, Mn, and Fe, 30 mL of 0.05 M Na12IP6 was mixed with 100 mL of 0.2 M HCl. A sufficient quantity of various metal chlorides was added to each of these solutions, so that a P to metal ratio of 1:1 was obtained in the reaction mixtures. The solutions containing Mg, Cu, or Mn chlorides were very carefully adjusted to a pH of 6 by slowly adding 1 M NaOH with stirring in 1-h time intervals (Evans and Pierce, 1982). In the same way, the pH of the solution containing Fe chloride was adjusted to pH 2 (Evans and Pierce, 1982). The pH of the solution containing Ca chloride was adjusted to 8.5 to assure proper precipitation of Ca IP6 compound (Graf, 1983). To prepare Al IP6 compounds, 30 mL of 0.3 M AlCl3 (pH 2.3) was added drop by drop to 30 mL of 0.05 M Na12IP6 (pH 11.0). The final pH of the reaction mixture was 2.4. An alternative Fe IP6 compound and a mixture of Al/Fe IP6 compounds were made following the same procedures described for Al IP6. The final pH of both reaction mixtures was 1.7. The prepared metal IP6 compounds were filtered and washed with 30 mL portions of boiling deionized water to remove any possible adsorbed or occluded metal ions (Evans and Pierce, 1982). These compound precipitates were air dried at room temperature, and then oven dried at 105°C for 1 h. For comparison, metal–orthophosphate complexes were prepared under same conditions with Na2HPO4 and metal chlorides. All products were kept in a desiccator at room temperature until use. Composition of these synthetic compounds was analyzed by the Analytical Laboratory of the Maine Agricultural and Forest Experimental Station. Total C content was run by combustion analysis on a Leco model CN-2000 (Leco Corp., St. Joseph, MI). Phosphorus and metal contents were run by dry ashing at 550°C to destroy any organic content, dissolving in 50% HCl, diluting, and analyzing the solutions by inductively coupled plasma–optical emission spectrometer (ICP–OES) (model 975) (Thermo Jarrell-Ash Corp., Franklin, MA).

Fourier Transform–Infrared Spectroscopy

The FT–IR of metal IP6 compounds were obtained using KBr discs. Each disc contained about a 1-mg sample and 80 mg of KBr. The spectra were recorded in the 450 to 4000 cm−1 range on a PerkinElmer Spectrum One FT–IR Spectrophotometer (PerkinElmer Instruments, Norwalk, CT). Each sample was scanned 24 times with a resolution of 2 cm−1. All spectra were normalized.

RESULTS AND DISCUSSION

Compositions of Metal IP6 Compounds

Evans and Pierce (1982) reported the preparation of IP6 compounds with Cu, Co, Fe, Mn, and Mg. They first obtained free phytic acid from Na salt of Na12IP6. They then mixed 20 to 30 mL of 0.05 M free phytic acid with 100 mL of 0.2 M KCl. In this way, the final IP6 solution was actually an acidified K–IP6 solution. Thus, the preparation of free phytic acid does not seem necessary. We simplified the procedure by directly mixing Na12IP6 with 0.2 M HCl to obtain an acidified Na–IP6 solution. The P/C mole ratios of the eight metal IP6 compounds ranged from 1:1.11 to 1:0.96 (Table 1), indicating that the structures of all six P–O–C bonds in IP6, (i.e., the identity of IP6), were not destroyed during the preparation process. The theoretic mole ratio of P to metal is 1:1 for metal(II)–IP6, and 1:0.67 for metal(III)–IP6. The actual ratios for Ca, Mg, Cu, and Mn IP6 compounds were close to stoichiometry (±10%) (Table 1). Evans and Pierce (1982) observed near stoichiometric ratios for Co–IP6 and Cu–IP6 (<10% difference). Other divalent metal compounds (Mg and Mn) contained less than stoichiometric metal contents. In our work, the P/Fe ratio in Fe–IP6–1 compound was 81% higher than stoichiometry, indicating some Fe hydroxide was present in the Fe–IP6 compounds. In contrast to our result, the P/Fe mole ratio (1:0.38) in the literature (Evans and Pierce, 1982; He et al., 2006b) was 43% lower than stoichiometry. This difference in stoichiometry may be related to the replacement of K with Na.

We further demonstrated that trivalent metal IP6 compounds could be made from unacidified Na12IP6 solution and metal chlorides. The P/Fe ratio in Fe–IP6–2 compounds was only 27% higher than stoichiometry. The stoichiometries in Al–IP6 and Al/Fe–IP6 were closer to the stoichiometry value of 1:0.67. The mole ratio of Al/Fe in Al/Fe–IP6 was 1:3, suggesting a preferential interaction between Fe ions and P–O bonds in IP6.

The purity of these synthetic compounds based on their P contents ranged from 66 to 82%. The lower purity implied that some crystalline water might have been present in these synthetic compounds. It is reported that each synthetic Mg6H2IP6 molecule contains 22 H2O molecules or 33.7% water (Torres et al., 2005). Metal (hydro)oxides could be another source of the low purity.

The theoretical mole ratio of P/metal is 1:1.5 for metal(II)–PO4 and 1:1 for metal(III)–PO4. None of the metal–PO4 complexes prepared reached the stoichiometry (Table 2). Whereas no insoluble Mg–PO4 was obtained, complexes with Ca, Cu, and Fe contained less than stoichiometry metal contents, indicating there still was some free phosphate group (P–O–H or Na) in these complexes. The more than stoichiometry metal contents

| Table 1. Compositions of synthetic metal phytate compounds. |
|-----------------|----------------|----------|---------------|----------------|-------|
| Metal–IP6       | C%             | P/C      | Metal         | P/C/Metal      | Purity§ |
| CaIP6           | 16.15          | 6.73     | 19.28         | 1:1.080:93     | 77.2   |
| MgIP6           | 17.07          | 7.33     | 12.95         | 1:1.110:97     | 72.9   |
| Cu2IP6          | 13.01          | 5.02     | 26.80         | 1:1.001:00     | 72.0   |
| Mn2IP6          | 15.53          | 6.63     | 27.40         | 1:1.010:100    | 81.6   |
| Fe2IP6–1§       | 14.06          | 5.47     | 30.74         | 1:1.011:21     | 65.9   |
| Al3IP6          | 17.7           | 6.54     | 10.95         | 1:0.950:71     | 72.0   |
| Fe3IP6–2§       | 15.23          | 6.19     | 23.44         | 1:0.950:85     | 71.3   |
| Fe2Al4IP6       | 15.59          | 6.42     | 17.30(Fe)     | 1:0.960:83     | 70.2   |

§ Prepared by directly adding FeCl3 into Na12IP6 solution.

‡ Prepared by adding NaOH into an acidified mixture of Na12IP6 and FeCl3.

™ Prepared by directly mixing Na12IP6 with 0.2 M HCl to obtain an acidified Na–IP6 solution.
Table 2. Compositions of synthetic metal orthophosphate complexes.

<table>
<thead>
<tr>
<th>Metal–PO₄</th>
<th>P</th>
<th>Metal</th>
<th>P/Metal</th>
<th>Purity†</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca₃(PO₄)₂</td>
<td>19.59</td>
<td>34.70</td>
<td>1:1.73</td>
<td>98.0</td>
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<tr>
<td>Mg₃(PO₄)₂</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Cu₃(PO₄)₂</td>
<td>14.39</td>
<td>40.92</td>
<td>1:2.84</td>
<td>76.2</td>
</tr>
<tr>
<td>Mn₃(PO₄)₂</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>AlPO₄</td>
<td>16.08</td>
<td>17.17</td>
<td>1:1.07</td>
<td>72.6</td>
</tr>
<tr>
<td>Fe₁₋ₓAlₓPO₄</td>
<td>16.39</td>
<td>17.94(Fe)</td>
<td>1:1.15</td>
<td>72.6</td>
</tr>
<tr>
<td>FePO₄·2H₂O</td>
<td>15.23</td>
<td>18.78</td>
<td>1:1.23</td>
<td>76.2</td>
</tr>
<tr>
<td>Fe₄₋ₓAlₓPO₄</td>
<td>16.39</td>
<td>17.94(Fe)</td>
<td>1:1.15</td>
<td>72.6</td>
</tr>
<tr>
<td>FePO₄</td>
<td>15.59</td>
<td>40.59</td>
<td>1:2.61</td>
<td>72.6</td>
</tr>
</tbody>
</table>

† Based on the difference in the P contents detected in the synthetic complexes and calculated from the theoretical formulas.
‡ No insoluble complex obtained.
§ Prepared by adding NaOH into an acidified mixture of Na₂HPO₄ and FeCl₃.
# Prepared by directly adding FeCl₃ into Na₂HPO₄ solution.

in Mn- and Al-containing complexes were due to preferential precipitation of metal hydroxides under the experimental conditions with the two metals. It is surprising that no excess ferric hydroxide was precipitated during the preparation of Fe complexes. The purities of metal orthophosphates were comparable to those of metal–IP₆ complexes, except for the high purity of Ca–PO₄.

Infrared Characteristics of Metal IP₆ Compounds

The FT–IR spectra of seven synthetic metal complexes and Na₁₂IP₆ are shown in Fig. 1. The spectrum of Fe–IP₆–1 is not shown because of its similarity to Fe–IP₆–2. All compounds showed a weak absorption band around 1680 cm⁻¹ and a broad absorption band at 3400 cm⁻¹ (data not shown). These two bands did not disappear when these samples were dried for 1 h at 105°C. The observations demonstrated the existence of O–H bonds (Celi et al., 1999; Chapman and Thirwell, 1964; Francioso et al., 1998) in these compounds, which could be due to the crystalline H₂O, metal hydroxide impurities, and unbounded P–O–H bonds.

Whereas one P–O bond is always connected to the C atom of a inositol ring, only two P–O bonds for each COPO₂ in IP₆ compounds are free to interact with either H or metals (Fig. 2). Each molecule of free acid IP₆ should contain six diprotonated monodeuterated tetragonal COPO₂. The characteristic infrared spectra of metal IP₆ compounds were from 1200 to 700 cm⁻¹ (Fig. 1). Celi et al. (1999) reported the spectral characteristics of KH₂₋₁IP₆, which is assumed to have five diprotonated and one monoprotonated COPO₂, to have a strong band at 991 cm⁻¹ and shoulder or weak bands at 1124, 1080, and 968 cm⁻¹. Each Na₃₋₂IP₆ had six COPO₂ nonsymmetrical tetragons. The spectrum of Na₃₋₂IP₆ showed a broad trailing band at 1106 cm⁻¹, triplet bands at 972, 937, and 913 cm⁻¹, and other triplet bands at 830, 776, and 740 cm⁻¹ (Fig. 1). Assuming that the broad band at 1106 cm⁻¹ represented three convoluted bands, the triplet characteristics implied three sets of COPO₂ (or C–O bonds) in Na₁₂IP₆. Each set was similar to that of dipotassium methyl phosphate (K₂H₃OPO₃) at 1095, 975, and 755 cm⁻¹ (Kumamoto, 1965) and aqueous HPO₄²⁻ at 1077, 989, and 850 cm⁻¹ (Arai and Sparks, 2001; Persson et al., 1996; Tejedor-Tejedor and Anderson, 1990). In other words, three different types of COPO₂ exist in Na₁₂IP₆ compounds. A 5-axial/1-equatorial structure of phytate has been proposed at alkaline solutions (Fig. 2A) (Barrientos and Murphy, 1996; Martin and Evans, 1986). We therefore suggest a similar structure is present in solid Na₁₂IP₆. Based on the relative spectral band strength and the number of symmetric P atoms, we assigned the FT–IR bands of 746 and 913 cm⁻¹ to P₁ and P₃, and 830 and 972 cm⁻¹ to P₁, P₄, P₅, and P₆. We grouped P₄, P₅, and P₆ because of the common feature that all three are flanked by opposite vertical P atoms on each side. Solution ³¹P NMR investigations have shown four peaks of aqueous IP₆ which distinguishes the six P atoms to four groups: P₂, P₁ and P₃, P₄ and P₆, and P₅ (Martin et al., 1987; Turner et al., 2003). FT–IR did not distinguish between P₄/P₆ and P₅, indicating less impact of far distance P atoms (P₂ to P₆ or P₁/P₃ to P₅) on P–O bond characteristics than on the magnetic resonance properties of P atoms.

The triplet characteristic in the spectra of synthetic divalent and trivalent metal compounds became obscure (Fig. 1). The minor absorption bands of Na₁₂IP₆ at 880 to 750 cm⁻¹ region were more like doublet bands and shifted upward 10 to 30 cm⁻¹ in these synthetic compounds. The sharp band at 972 cm⁻¹ shifted to 996 cm⁻¹ with Ca–IP₆, and 1010 cm⁻¹ with Mg–IP₆. Both compounds showed the broad band around 1135 cm⁻¹ with less trailing character. In the spectra of Cu and Mn compounds, the broad band split into two overlapped but distinguishable bands at 1086 cm⁻¹ and 1133 cm⁻¹ or nearby with the sharp band at 997 cm⁻¹. The spectral characteristics of trivalent metal (Fe and Al) compounds included a shoulder band at 1007 cm⁻¹ with a strong band at 1092 or 1166 cm⁻¹. The spectra of Al/Fe IP₆ were similar to those of Fe or Al compounds. These observations reflect the structural differences among those synthetic compounds.

Whereas further data are needed to elucidate the specific structures of these synthetic metal IP₆ compounds, the general trend of upshifting wave numbers, compared to those of Na₂HPO₄, reflects the increased interactions between metal ions and P–O bonds in IP₆. Martin and Evans (1986) have reported that all phosphate groups in IP₆ lose a proton before second dissociation steps occur. They proposed two Ca(II)–IP₆ structures in which a Ca(II) ion coordinates with two O atoms in two separate COPO₂ groups, rather than with two O atoms in one single COPO₂ group. Similarly, we proposed possible structures of metal(II)–IP₆ compounds with COPO₂ groups (Fig. 2B). A possible structure of metal(III)–IP₆ was constructed in the same way (Fig. 2C). Near 3:1 ratio of Fe/Al in Fe/Al–IP₆ compound could be partly explained by the integer of metal ions in this structure in Fig. 2C. It should be noted that the original structure of 5-axial/1-equatorial chair structure in Na₁₂IP₆ could be distorted due to interlocking forces among COPO₂ groups and multiple valent cations, even though it is not clearly indicated in Fig. 2B and 2C. The interlocking forces were evident by the change of triplet bands to doublet bands at 880 to 750 cm⁻¹ region. In the extreme case, a boat struc-
ture of IP6 binding on αFeOOH has been proposed (Celi et al., 2001).

Infrared Characteristics of Metal Phosphate Compounds

Metal orthophosphates showed the different FT–IR spectral characteristics from their IP6 counterparts (Fig. 3). This is because of the monophosphoester bonds (P–O–C) in IP6. The restrain effect of inositol ring which has P clustered in six might have also played some roles. The peak of Na₃PO₄·12H₂O (1011 cm⁻¹) was closer to 1006 cm⁻¹ of aqueous PO₄³⁻ (Arai and Sparks, 2001) than 960 cm⁻¹ of Ag₃PO₄ (Rulmont et al., 1991), indicating a similar tetrahedron structure in these compounds. Spectra of synthetic divalent Ca and Cu phosphates seem the combinations of the band (strong) of aqueous PO₄³⁻ and three bands (weak) of aqueous...
HPO$_4^{2-}$ (Arai and Sparks, 2001) which implied that whereas most of synthetic Ca and Cu phosphate compounds were tribasic salts, with some of them in dibasic forms. Very complicated with about eight bands appeared in the same region in the spectrum of synthetic Mn phosphate compounds. It is reported that LaPO$_4$ with four distorted ions in a monoclinic cell shows quadruplex bands at 640 to 500 cm$^{-1}$ and 990 to 1100 cm$^{-1}$ regions with an additional band at 950 cm$^{-1}$ (Rulmont et al., 1991). Thus, we believe, similar to the case of LaPO$_4$, multiple distorted PO$_4$ ions might have been in the Mn phosphate compound. All the trivalent metal phosphates had a single broad band around 1050 cm$^{-1}$ (Fig. 3). The peak of AlPO$_4$ had the higher wave number than that of FePO$_4$, and that of the mixture was between the two. This observation was consistent with that derived from Fe and Al IP6 compounds. Thus, the peak at different wave numbers may be useful in differentiating Al from Fe P compounds.

**Fig. 2. Possible molecular structures of metal phytates.** (A) Ionic 5-axial/1-equatorial conformation associated with Na$^+$. For clarity, metal bondings are only shown on P5. (B) M$^{2+}$ coordinate bonding conformations. (C) M$^{3+}$ coordinate bonding conformation.

**Distinction of Metal Phosphorus Species by FT–IR Analysis**

Infrared spectroscopy has been used extensively to identify soil constituents and to elucidate structural features of both inorganic and organic components (John-
So does in characterization and the structural study in phosphate species (Chapman and Thirlwell, 1964; Tejedor-Tejedor and Anderson, 1990; Rulmont et al., 1991; Arai and Sparks, 2001). The differential FT–IR spectra among different types of metal phosphates and phytates imply the possibility to distinguish these compounds by FT–IR analysis. That is, the reference spectra in Fig. 1 would be of diagnostic value for the identification of different types of metal phytates. For this purpose, we further examined the IR features of several mixtures of these compounds. The major broad bands and their shoulders in all three spectra of the mixtures of two types of phytate compounds were like the summation of the relevant spectral bands of the two individual compounds (Fig. 4). In other words, the spectrum of each mixture was simply an assemblage of the two

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Fig. 3. Fourier transform infrared spectroscopy (FT–IR) of trisodium phosphate dodecahydrate and the synthetic metal phosphate compounds.
separate spectra. This observation indicates that a complicated FT-IR spectrum of phytate mixtures could deconvolute to the contribution of individual compounds using peak deconvolution and Gaussian profile fitting treatments (Arai and Sparks, 2001).

Similarly, spectra of the mixtures of metal phosphates and sodium phytate had the features of both the orthophosphate and sodium phytate (Fig. 5). Whereas those major bands beyond 1000 cm\(^{-1}\) were more similar to those of individual metal phosphate, the spectral features from 1000 to 700 cm\(^{-1}\) were those of sodium phytate. Thus, except for the mixture of Mn phosphate, the bands around 990 and 830 cm\(^{-1}\) could be used to as an indicator of Na phytate in these metal phosphate compounds. To identify the Na phytate mixing with Mn phosphate, the feature of all three bands of Na phytate at 863, 771, and 746 cm\(^{-1}\) should be taken in consideration. Although not shown in this work, this obser-
vation could be applicable to the mixtures of metal phosphate with other metal phytate compounds because all phytate compounds have the unique FT–IR bands around 830 cm$^{-1}$.

Our observations indicate that different metal species of phosphate and phytate compounds have their unique FT–IR features which may be of diagnostic value for the identification of different types of phosphates. Although it is questionable whether the FT–IR analysis can be used to analyze P species in real world samples due to the low P concentration in these samples and interfering bands of other chemical groups in the same region (such as C–O stretching of polysaccharide) (Johnston and Aochi, 1996), we believe that at least FT–IR analysis after fine tuning could provide an analytical tool to investigate the basic metal phytate chemistry in molecular levels, such as the competitive interactions between phosphate and phytate with a specific metal ion, and the

Fig. 5. FT–IR spectra of the mixtures of trisodium phosphate dodecahydrate and the synthetic metal phosphate compounds with dodecasodium phytate.

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conversion (or hydrolysis) of metal phytate to metal phosphate under various conditions. Such fundamental research might shed light on possible interactions and transformations of metal–phytate species in the environment. For instance, both Ca and Mg are reported to play significant roles in solubility of poultry litter P (Cooperband and Good, 2002; Nair et al., 2003). The Al- and Fe-contained chemicals or by-products have been proposed to stabilize manure P to reduce runoff P (Dou et al., 2003; Moore et al., 2000). These investigations have mainly focused on inorganic P, but more recent studies have shown a significant portion of manure P to be organic P, primarily in the phytate form (He et al., 2004a, 2004b, 2006a; Jayasundera et al., 2005). We hope that basic knowledge of phytate chemistry yielded from this and other studies (Dao, 2003, 2004b; He et al., 2006b; Seaman et al., 2003) will improve and promote research on the fate and bioavailability of phytate in the environment, which is determined not only by the indigenous dephosphorylating activity (Seeling and Jungk, 1996; Tarafdar and Claassen, 1988; Yadav and Tarafdar, 2003), but also by the degree of interactions with metal species.

CONCLUSIONS

Eight metal–phytate compounds were synthesized from Na12IP6 and metal chlorides. Elemental analysis indicated that compounds with Ca, Mg, Cu, Mn, Al, and Al/Fe were obtained near stoichiometry (±10%). The P/Fe ratios in the Fe–IP6 compounds were higher than stoichiometry, indicating the presence of Fe hydroxide in the Fe–IP6 compounds. FT–IR spectroscopy revealed the differential spectral features of these synthetic compounds, which could be used to classify metal phytate compounds into three groups: (i) light divalent metal (Ca and Mg) phytate compounds with a sharp band and a broad band, (ii) heavy divalent metal (Cu and Mn) compounds with splitting broad bands, and (iii) trivalent metal compounds with a broad band and a shoulder band. The unique FT–IR features of different metal species of phosphahte and phytate compounds may be of diagnostic value for the identification of different types of phosphates.

REFERENCES


