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Infrared Spectroscopy in the Analysis of Building and Construction Materials

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In memorial of Prof. Tomás Vázquez

1. Introduction

In the characterization of building and construction materials, the most frequently analytical tool performed have been X-ray diffraction but also, thermal analysis and microscopic techniques. Nowadays, infrared and other spectroscopic techniques have become as a useful, non-destructive and easy technique to study the phase composition of initial but also the evolved materials due to their exposure to the climatic conditions. Moreover, by using this tool is possible the detection of crystalline but also the amorphous phases very frequently developed on certain cementitious materials, mainly at early ages. The infrared spectroscopy is used both to gather information about the structure of compounds and as analytical tool to assess in qualitative and quantitative analysis of mixtures.

The infrared spectra are quick and easy to achieve and refers to the spectrum region between the visible and microwave regions. In theory, infrared radiation is absorbed by molecules and converted into energy of molecular vibration; when the radiant energy matches the energy of a specific molecular vibration, absorption occurs. The frequencies at which a molecule absorbs radiation give information on the groups present in the molecule. As an approximation, the energy of a molecule can be separated into three additive components associated with the motion of the electrons in the molecule, the vibration of the constituent atoms, and the rotation of the molecule as a whole. The absorption in the infrared region arises predominantly from excitation of molecular vibrations. Then, if a molecule is placed in an electromagnetic field, a transfer of energy from the field to the molecule will occur when Bohr's frequency condition is satisfied.

$$\Delta E = h\nu$$

Where ΔE is the difference in energy between two quantized states, h is the Planck's constant and ν is the frequency of the light. Then the molecule "absorbs" ΔE when it is excited from $E_1$to E_2 and "emits" ΔE when it reverts form E_2 to E_1. The infrared absorption spectra originate in photons in the infrared region that are absorbed by transitions between two vibrational levels of the molecule in the electronic ground state.

The application of infrared spectroscopy to the inorganic compounds started as a more frequent technique during the 60's with Lawson. This author made a first attempt to compile the work done in the relatively new field-Inorganic Infrared Spectroscopy since 1952 where 1171 references were reported. Farmer, in 1964, studied the silicates and Nakamoto in relation to the coordinated compounds prepared a helpful atlas of these compounds. Afremow (1966) presented for an important research of inorganic pigments and extenders in the mid-infrared region from 1500 cm-1 to 200 cm-1. The study of surface chemistry and the nature of surface functional groups was also advanced by Basila (1968).

In the first decade of infrared research on the study of Portland cements, Vázquez (1969), was a lead the way in the study by infrared spectroscopy the main present compounds in the Portland cement but also later, made some research about the carbonation processes of calcium aluminate cements. Also, the hydration of Portland cement and its constituents was developed by Bensted (1974).

After that initial period, several reports have been done in the study on cementitious materials by infrared. More recent studies in relation with the calcium aluminates cements were reported by Vázquez (1993). Later on, different papers have present some characterization of materials and evolution over several exposition conditions using the infrared spectroscopy as a complementary technique join to mainly XRD and SEM analytical tools.

Without doubt, the infrared spectroscopy has not been really used in the qualitative and quantitative analysis of these materials; the main uses have rather been in identification of compounds and few structural studies. The main objective of this chapter will be to present a revision of infrared spectra useful in the study of the building and construction materials, mainly cements, from the point of view of characterization.

2. Characterization of cementitious systems by infrared spectroscopy

As a general rule, as it is easier to bend a bond than to stretch or compress it, in the spectra the stretching frequencies are higher than the corresponding bending frequencies; bonds to hydrogen have higher stretching frequencies than those to heavier atoms; and double bonds have higher stretching frequencies than single bonds (Figure 1).

2.1 Portland cement

The ordinary Portland cement is made by firing raw materials - limestone, clay minerals, sand and iron minerals- at around 1500ºC in a rotary kiln. At this temperature a series of chemical reaction take place and the clinker synthesized. Clinker is cooled, mixed with setting regulators (e.g. gypsum) grounded to a fine powder to obtain the cement. The common phases present in the cement clinkers are: alite ($3CaO \cdot SiO_2$, C_3S[1]), belite ($2CaO \cdot SiO_2$, C_2S[1]), tricalcium aluminate ($3CaO \cdot Al_2O_3$, C_3A[1]), and tetracalcium aluminate ferrite ($4CaO \cdot Al_2O_3\, Fe_2O_3$, C_4AF[1]). One typical composition of cement consists of: C_3S = 55-60% (wt); C_2S = 15-20% (wt); C_3A = 5-10% (wt); C_4AF = 5-8% (wt) and $C\bar{S}H_2$ = 2.6% (wt). In this chapter, synthetic silicates and aluminates phases have been used to identify infrared vibrations bands previous to study the more complicated commercial cement.

[1] Cement chemistry nomenclature is used: $C = CaO$; $S = SiO_2$; $A = Al_2O_3$; $F = Fe_2O_3$; $H = H_2O$; $\bar{S} = SO_3$

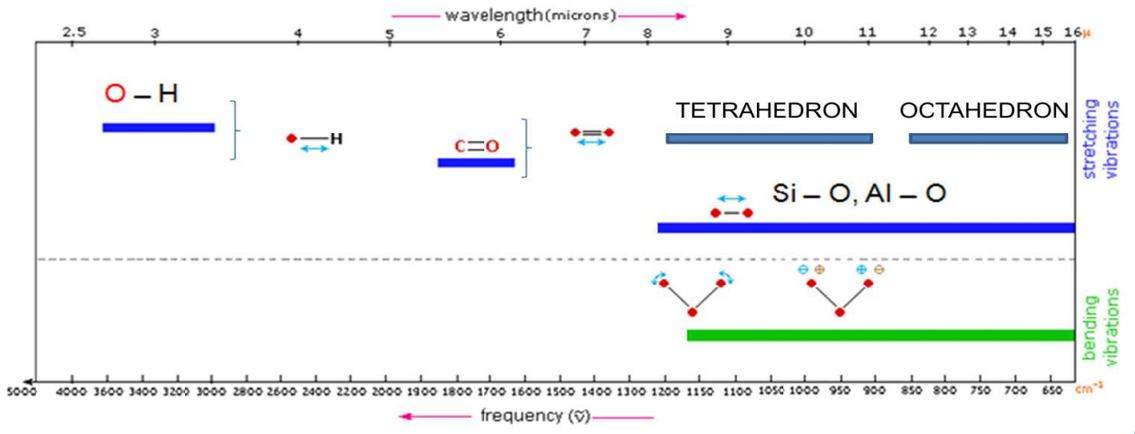


Fig. 1. General rules in the interpretation of building cementing material IR spectra.

As a resume, the vibrations can be divided in stretching and bending: vibrations can involve either a change in bond length (stretching) or bond angle (bending); some bonds can stretch in-phase (symmetrical stretching) or out-of-phase (asymmetric stretching). The main structure elements in building the crystal lattice of silicates are tetrahedral SiO_4 groups, with may be either isolated as in the orthosilicates or connected with one another by common O atoms as in building an Si_2O_7 group from two connected tetraheda [Matossi]. Connection of SiO_4 groups so as to form a ring of tetrahedral occurs in the crystal of alite (C_3S) or belite (C_2S). The infrared spectra of all silicates [Matossi] contain two reflection maxima near 1000 and 500 cm^{-1}, which have been interpreted as a two active frequencies of a tetrahedral point group. In addition to these, there may occur other maxima corresponding to other particular features of the crystal lattice.

The spectrum of the main constituent of OPC, C_3S, shows two regions dominated by the internal modes of SiO_4^{4-} tetrahedral units, with to broad absorption bands centred between 890 and 955 cm^{-1}, solved in to maxima near to 870 and 940 cm^{-1} due to the symmetric and antisymmetric stretching of Si-O bonds within tetrahedral SiO_4 groups, ν_1 and ν_3, respectively. Another absorption band of medium intensity appears close to 525 cm^{-1} and a lower intense band sited near to 450 cm^{-1} due to the symmetric and antisymmetric bending of the O-Si-O bonds, ν_2 and ν_4, respectively (see details of maxims in Table 1 and Figure 2). The other calcium silicate phase spectra, C_2S, exhibits strong bands in the area 1000-800 cm^{-1} with maximums at 990 and 840 cm^{-1} due the stretching Si-O bond of the silicon tetrahedron and the bending vibration absorption band appear at lower frequencies, 520 cm^{-1} and a shoulder at 538 cm^{-1}.

The C_3A-cubic tricalcium aluminate polymorph spectra (Figure 3), shows a well-defined spectra with two dominant absorption areas with very broad bands. The first ones appear in the area between 950-650 cm^{-1} and the second ones appearing between 500-380 cm^{-1}, respectively. The main observed maxima appear near to 900, 865, 820, 780, 720 and 705 cm^{-1} of AlO_4-tetrahedral groups, and close to 520, 510, 460 and 414 cm^{-1} due to AlO_6-octahedral groups. The Ca-O bands appear at lower frequencies.

The grey colour of Portland cements is due to the presence of the names ferrite phases; in absence of elements other than calcium, aluminium, iron and oxygen, calcium

phase	Fundamental vibrations (cm^{-1})	
C_3S	935	521
$\beta - C_2S$	991, 879, 847	509
C_3A	900, 865, 820, 780, 720, 705	520, 510, 460, 414
C_4AF	700 - 500	

Table 1. Characteristic absorbance bands for cement Portland phases

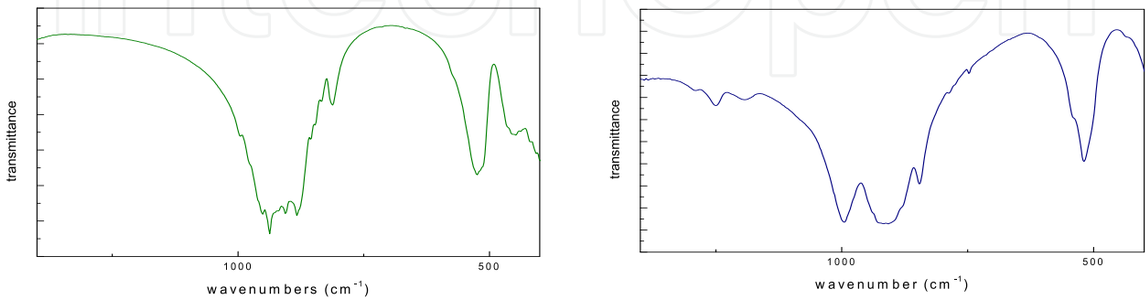


Fig. 2. Infrared spectra of pure C_3S (left) and C_2S (right).

aluminoferrite forms a solid solution series of formula $Ca_2(Al_xFe_{1-x})_2O_5$ for all values of x in the range 0-0.7, compositions with x > 0.7 do not exist at ordinary pressures. The spectrum of C_4AF presents as significant absorption bands the sited between 800-830 cm^{-1} with maxima close to 720 cm^{-1} due to ν_1 [$(Fe,Al)O_4^{5-}$]; moreover, a broad and less intense band with several maximums between 620 and 670 cm^{-1} is also present (Figure 3).

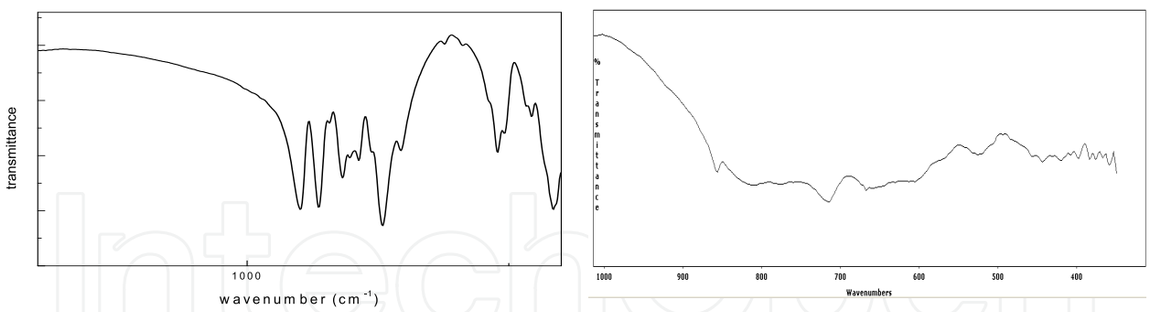


Fig. 3. Infrared spectra of C_3A (left) and C_4AF (right).

In a real cement the main phases are alite (C_3S-base solid solutions i.e. MgO, Na_2O) and belite (C_2S-base solid solutions i.e.- Al_2O_3, Fe_2O_3). The presence of these impurities prompts a change in the crystalline structure of the silicate phases that may cause modifications in the Infrared spectra compared to the pure phases. Figure 4 present the infrared spectra of the ordinary Portland cement. In this spectrum, it is possible to identify different vibrations bands from the calcium silicates, calcium aluminates, and gypsum, the last one added as setting regulator.

The gypsum can lose part of the structure water and the sulfates can be present as bassanite and/or anhydrite. In the IR spectras, the strongest peak is presented at 1102, 1111, and 1094

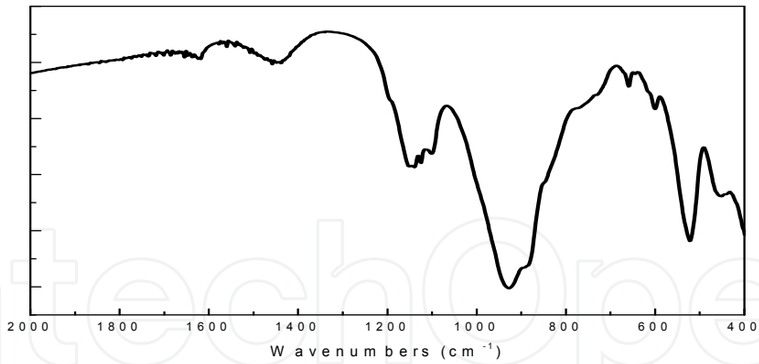


Fig. 4. IR Spectrum of ordinary Portland cement.

cm^{-1}, for the gypsum, bassanite, and anhydrite, respectively. They are ν_3 antisymmetric stretch vibration modes of SO_4 tetrahedra. The gypsum, bassanite, and anhydrite present two absorption bands (669, 604 cm^{-1}), three **(**660, 629, 600 cm^{-1}) and three (677, 615, 600 cm^{-1}), anti-symmetric bending vibrations, respectively. The peaks at 595 cm^{-1} in gypsum and 594 cm^{-1} in bassanite split into two peaks (610 and 591 cm^{-1}) in anhydrite, which indicates a lowering of symmetry in anhydrite. The shift of frequency from 677 cm^{-1} in anhydrite to 660 cm^{-1} in bassanite indicates that the sulfate ions in bassanite are linked with water molecules by hydrogen bonding, because in general the hydrogen bonding will lower the frequency of the absorption band. In addition, there is a very weak peak at 1140 cm^{-1} in gypsum, 1150 cm^{-1} in bassanite, and 1150 cm^{-1} in anhydrite, which should be the ν_1 symmetric stretch vibration modes of SO_4 tetrahedral. The Table 2 present the characteristics absorption bands of sulfate compounds. For gypsum and bassanite presence it will be also possible to analyze 4000-3000 cm^{-1} region were ν_1 O-H absorptions can be observed (3553 and 3399 cm^{-1} for gypsum and 3611 and 3557 cm^{-1} for bassanite).

Sulfates	FUNDAMENTALS			OVERTONES	OH-STRECHT	OH-BEND
	ν_1	ν_3	ν_4			
gypsum	1140	1117	669, 604	2500 - 1900	3553, 3399	1686, 1618
Bassanite	1150	1117, 1098	660, 629, 600	2500 - 1900	3611, 3557	1618
anhydrite	1150	1120	677, 615, 600	2500 - 1900	---	---

Table 2. Absorption bands of sulfate compounds (cm^{-1})

2.2 Calcium aluminate cement

The calcium aluminate cement (CAC) was developed as a solution to the sulphates attack in OPC, and was patented in France in 1908. The CACs are cements consisting predominantly of hydraulic calcium aluminates: mainly monocalcium aluminate, CA, but also contains minor amounts of $C_{12}A_7$, CA_2 and C_4AF.

According to Tarte, in the interpretation of IR spectra of inorganic aluminates, the characteristic frequency ranges are "condensed" AlO_4 tetrahedral in the 900-700 cm^{-1}, "isolated" AlO_4 tetrahedral 800-650 cm^{-1}, "condensed" AlO_6 octahedral in the 680-500 cm^{-1},

"isolated" AlO_6 octahedral 530-400 cm^{-1}. In the spectra of the main present phase of CAC, the CA, the most relevant signals are presented in the two region 850-750 cm^{-1} and 750-500 cm^{-1} due to the mentioned groups, with maxima near to 840, 805, 780 and 720 cm^{-1} of AlO_4 tetrahedral and close to 680, 640, 570, 540, 450 and 420 cm^{-1} of AlO_6 groups (Figure 5).

The infrared spectrum of $C_{12}A_7$ contains absorption bands mainly in two regions: a very broad absorption region between 680-900 cm^{-1} of tetrahedral groups and another area in the 650-400 cm^{-1} range with very sharp and intense bands due to octahedral groups. The maxima appear close to 850, 780, 610, 575, 460 and 410 cm^{-1} (Figure 5).

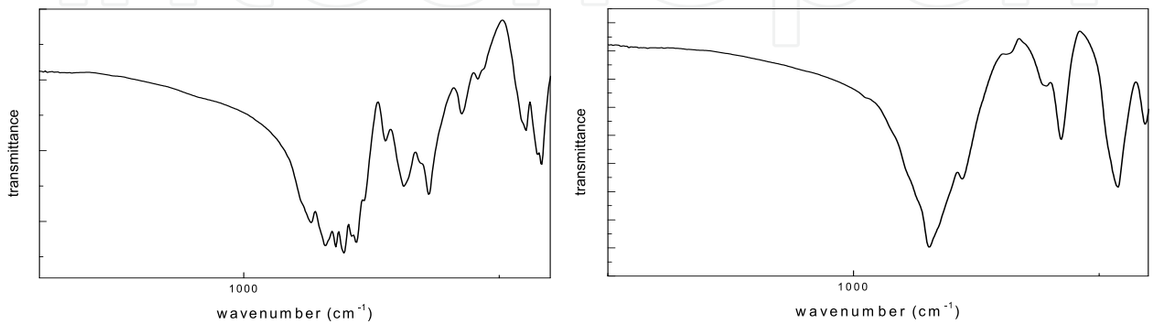


Fig. 5. Infrared spectra of CA (left) and $C_{12}A_7$ (right).

The minor phases present in the CAC are the CA_2 aluminate with the two absorption in the areas 950-700 cm^{-1} and 690-410 cm^{-1} with maxima at 945, 920, 860, 840, 810 and 745 cm^{-1} of AlO_4 groups and near to 680, 660, 640, 575, 540, 440 and 422 cm^{-1} of AlO_6 groups. The C_2AS mineral presents the AlO_4 vibration area between 920 and 720 cm^{-1} while the AlO_6 groups give absorption bands between 720-400 cm^{-1}. At higher frequencies, in this spectra appear the signals due to the Si-O vibrations, 1020 and 973 cm^{-1}. The IR spectra of CA_2 and C_2AS are presented in Figure 6.

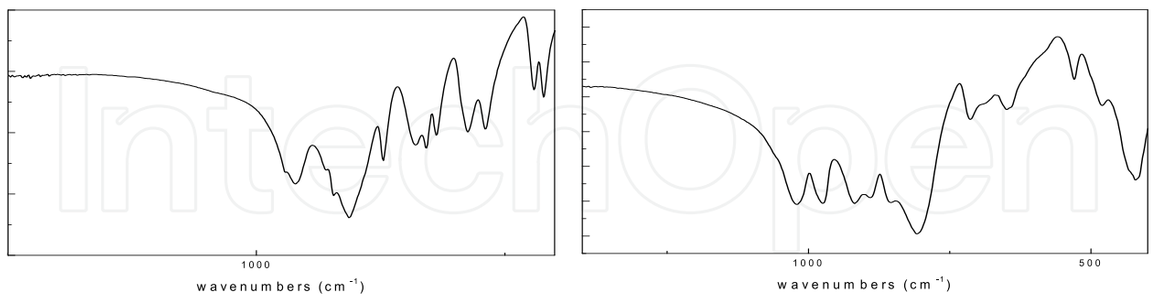


Fig. 6. Infrared spectra of CA_2 (left) and C_2AS (right).

Then, the most relevant signals on the FTIR spectrum for CAC are the absorption bands in the region between 850 and 650 cm^{-1} – the bands at around 840, 805 and 780 cm^{-1} – attributed to AlO_4 groups; the bands between 750 and 400 cm^{-1} – with bands at about 720, 685, 640 and 570 cm^{-1}, ascribed to AlO_6 groups; and the bands at under 400 cm^{-1} owing to Ca-O bonds [15, 16]. The Figure 7 shows the IR spectra of the commercial cement. The Table 3 presents the characteristics absorption bands of CAC mineral compounds.

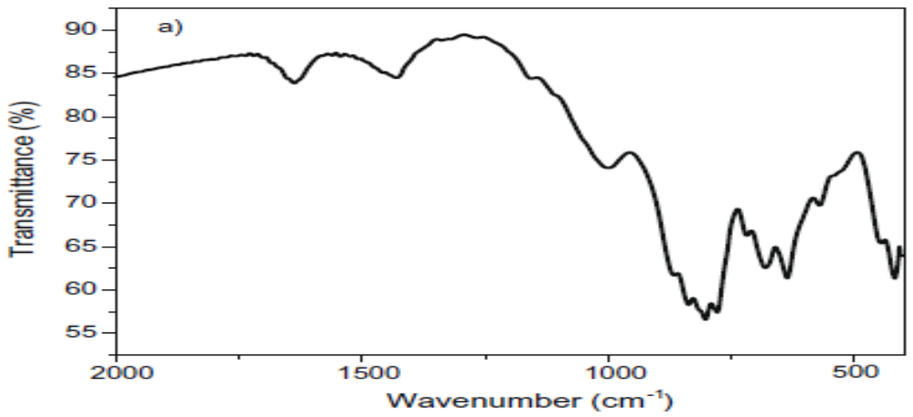


Fig. 7. IR spectra of commercial calcium aluminate cement.

phase	Fundamental vibrations (cm^{-1})	
CA	840, 805, 780, 720	680, 640, 570, 540, 450, 420
$C_{12}A_7$	850, 780,	610, 575, 460, 410
CA_2	945, 920, 860, 840, 810, 745, 680,	660, 640, 575, 540, 440, 422
C_2AS	920, 720, 710, 1020, 973	650, 530, 480, 420

Table 3. Characteristic absorbance bands for calcium aluminate cement phases.

2.3 Calcium sulfoaluminate cement

From the sustainability point of view new cement production has been developed in the past decades. One of these new cements is calcium sulphoaluminate (CSA) that was first developed in China in1980´s. Industrial production requires essentially gypsum, bauxite and limestone as raw materials, which are burnt at 1,300ºC in a conventional rotary kiln. These starting materials lead to a final clinker based on the quinary system CaO–SiO_2–Al_2O_3–Fe_2O_3–SO_3 and formed by three main minerals: tetracalcium trialuminate sulphate or yeelimite ($C_4A_3\bar{S}$); dicalcium silicate or belite (C_2S) and calcium sulphate or anhydrite ($C\bar{S}$). Minor phases such as C_3A, C_4AF, $C_{12}A_7$ and (C_2AS) can also be present. The infrared spectra of main mineral phase of calcium sulphoaluminate cement can be described as follow: yeelimite has two absorption bands due to vibrational modes of sulphate $[SO_4]^{2-}$ groups at 1110 cm^{-1}, a very intense absorption band due to silicate groups near to 800 cm^{-1}, the third band at 620 cm^{-1} is due to vibrational modes of $[AlO_4]^{5-}$ tetrahedra; ii) belite, anhydrite, $C_{12}A_7$ and C_2AS spectras have been described previously. Then, the infrared spectrum of the CSA cement presents the most intense bands located at 1110 and 800 cm^{-1}, in the region where stretching vibrations of $[SO_4]^{2-}$ groups lie. A broadened signal appears between 900 and 800 cm^{-1}, centered at 857 cm^{-1}. This feature is strongly asymmetrical: this is probably the result of the convolution of the two bands of C_2S, that appear unresolved or as a consequence of lower crystal perfection caused by the presence of foreign ions in the lattice or because of the small particle size of minerals of CSA clinker. But it is also possible to highlight the presence of the three anhydrite bands at 677, 615, and 600 cm^{-1}, respectively. The Figure 8 displays the IR spectra of yeelimite.

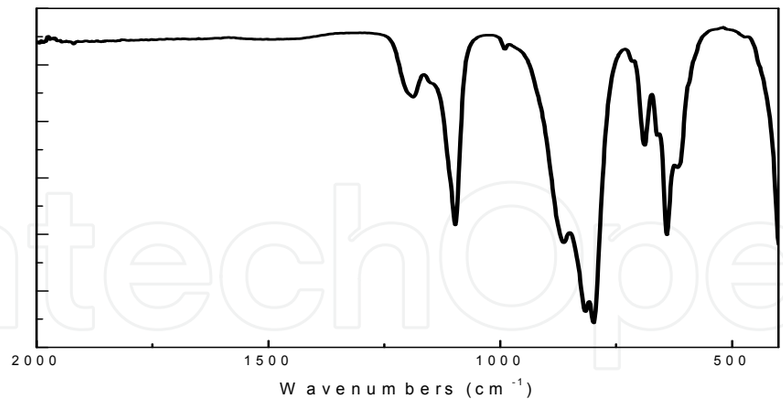


Fig. 8. Infrared spectra of yeelimite.

3. Infrared analysis of hydrated cementitious materials

The hydration of Portland cement give rise both, amorphous phase calcium silicate hydrated (C-S-H gel) and two crystalline phases, ettringite ($Ca_6Al_2(OH)_{12} \cdot (SO_4)_3 \cdot 26H_2O$) and portlandite. The C-S-H gel is the primary binding phase in Portland cement but poorly crystalline. The Figure 9 presents the infrared spectra of a hydrated commercial Portland cement.

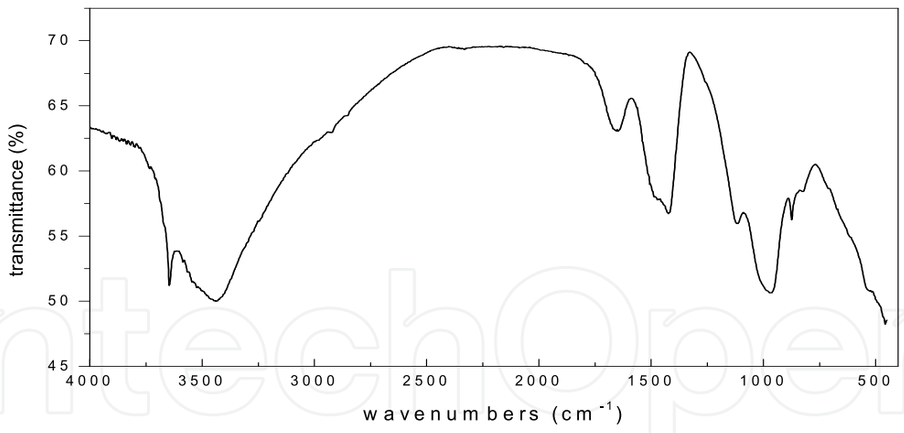


Fig. 9. IR spectra of hydrated Portland cement.

The ettringite ($C_6A\bar{S}H_{32}$) is the first developed phase due to the reaction of aluminates with sulfates of Portland cement. According to the structure model by Taylor [76], the crystals are based on columns of cations of the composition $\{Ca_3[Al(OH)_6] \cdot 12\ H_2O\}^{3+}$. In there, the $Al(OH)_6^{3-}$-octahedral are bound up with the edgesharing CaO_8-polyhedra, that means each aluminum-ion, bound into the crystal, is connected to Ca^{2+}-ions, with which they share OH^- ions. The intervening channels contain the SO_4^{2-}-tetrahedral and the remaining H_2O molecules (fig. 2). The H_2O molecules are partly bound very loose into the ettringite structure. According to Bensted, the infrared spectra of ettringite $C_3A \cdot 3C\bar{S} \cdot H_{32}$ or

$Ca_6[Al(OH)_6]_2(SO_4)_326H_2O$ presents a very strong anti-symmetrical stretching frequency of the sulphate ion (ν_3 SO_4) centred towards 1120 cm^{-1}; this band is indicative of relative isolation of this ion in the hexagonal prism structure. The water absorption bands appear in the region 1600-1700 cm^{-1} (1640 and 1675 cm^{-1} ν_2 H_2O) and above 3000 cm^{-1} (3420 due to ν_1 H_2O and 3635 cm^{-1} from ν OH_{free}). The presence of aluminate bands are near to 550 cm^{-1} (ν AlO_6) due to stretching Al-O groups, and 855 cm^{-1} (Al-O-H bending). The Figure 10 shows the structure and the infrared spectra of ettringite compound.

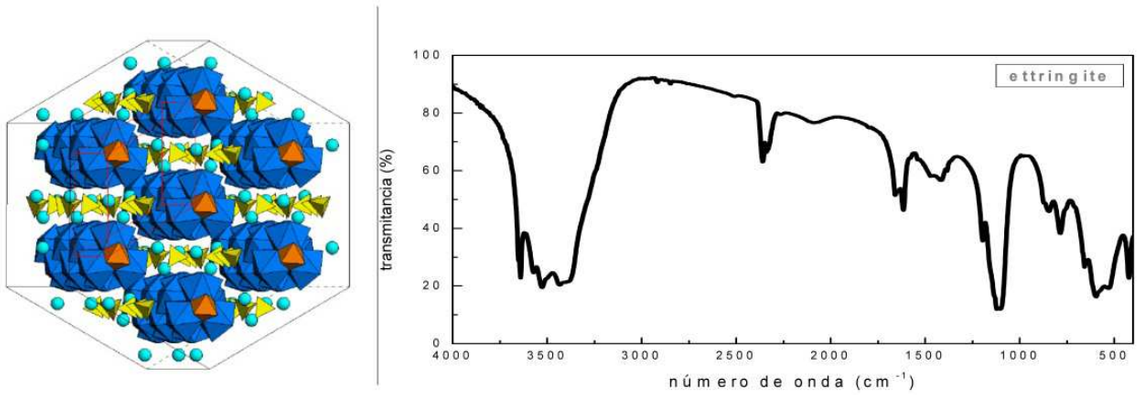


Fig. 10. Structure model of ettringite (according to Dr. J. Neubauer/University Erlangen/ Germany) (left), infrared spectra of ettringite (right).

The other crystalline phase present in cement hydration, *portlandite, $Ca(OH)_2$*, shows two prominent sharp peaks, the first one at 3645 cm^{-1}due to the presence of OH stretching and the second one at 353 cm^{-1}assigned to Ca-O lattice vibrations (Figure 11).

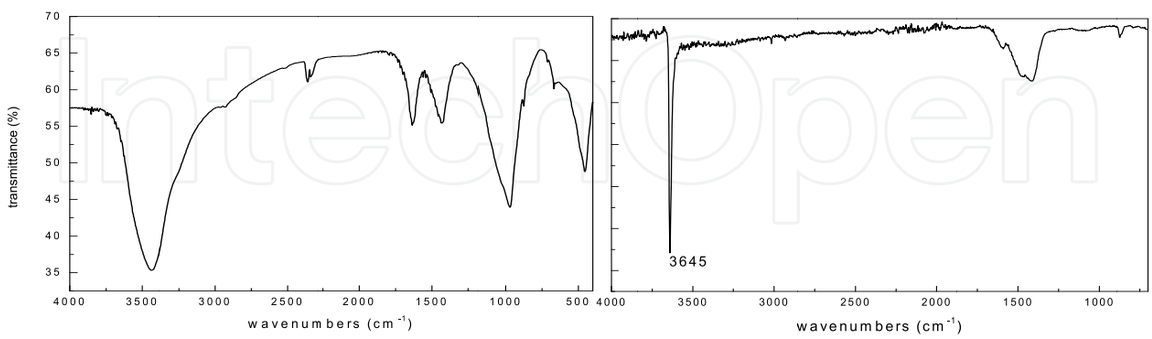


Fig. 11. Infrared spectra of gel C-S-H (left) and portlandite (right)

While crystalline materials give sharp well-defined bands and the glasses give broad, poorly defined bands, the C-S-H samples lie between these two extremes. The distribution function, which describes the line shape of the bands, is strongly dependent upon the

distribution of bond angles and bond lengths within common environments, and the broad half-width of the absorption bands of the C-S-H samples reflect their low symmetry and crystallinity. This distribution is assumed to be symmetry for glasses; hence, any asymmetry of the shape of the bands is due to a superimposition of several symmetrically shaped bands. The infrared spectra of synthetic *C-S-H gel* samples show a broad band in the 3800-3000 cm^{-1} region attributed to OH stretching vibrations of water molecules with maxima close to 3420 and 3626 cm^{-1}, 1428 and 666 cm^{-1}(Figure 11). According to Martinez-Ramirez, depending on the C/S ratio of the C-S-H gel the frequency of the maximum can be different.

With respect to the *CACs*, the normal CAC hydration with water gives up to the development of hydrated calcium aluminates, CAH_{10} at low temperatures but C_2AH_8 and C_3AH_6 at intermediate and high temperatures joint to AH_3 according to the following reactions:

$$CA + 10H \longrightarrow CAH_{10} \quad (1)$$

$$2CA + 11H \longrightarrow C_2AH_8 + AH_3 \quad (2)$$

$$3CA + 12\,H \longrightarrow C_3AH_6 + 2AH_3 \quad (3)$$

High early strength, good chemical resistance and high temperature resistance of calcium aluminate cement (CAC) products had encouraged the use of CAC in certain applications. However, conversion of hexagonal phases, CAH_{10} and/or C_2AH_8 to cubic C_3AH_6 and AH_3 in hydrated CAC cement under certain temperature conditions has been the major consequence in limiting its use to special applications. The presence of a minor amount of C_2ASH_8 (strätlingite) in CAC at later ages may be responsible of some strength recovery after conversion process.

The IR spectra of CAH_{10} have a very broad and intense band due to hydroxyl vibration in the 3400-3550 cm^{-1} region, with maxima near to 3500 cm^{-1}. A very weak band at 1650 cm^{-1} is associated to the H-O-H deformation vibration. The 1200-400 cm^{-1} region is a very poor resolution area due to the complexity and associated vibrations sometimes indicating a low crystalline grade; but some absorption bands at 1,024, 774 (shoulder) 699 and a doublet close to 573-528 cm^{-1}. The IR spectra of the CAH_{10} phase are depicted in Figure 12. *The β-C_2AH_8 hexagonal phase presents in the* 3400-3700 cm^{-1} region absorption bands at 3,465 and 3,625 cm^{-1} due to OH vibrations of the molecular water. In the 1100-400 cm^{-1} region there is a very complex vibration area with difficulties in the interpretation.

The *C_3AH_6* and the gibbsite are the stable phases in this system. The C_3AH_6 structure can be described as $[Al(OH)_6]^{2-}$ octahedrals connected by Ca^{2+} cations. The IR spectra presents a very intense OH-free band at 3670 cm^{-1}. This compound do not presents water molecular in the structure so, in the area between 3,400 and 3,600 cm^{-1}, there is not the presence of the deformation H-O-H band. Others fundamental bands due to the stretching and bending vibrations of the Al-O in the octahedral AlO_6 groups, appear at 802, 525 and 412 cm^{-1} (Figure 12).

Different AH_3 polymorphs can be identified by FTIR (Table 4). Although the differences in the strength of OH bond are reflected mainly by the numerous absorption maxima in the

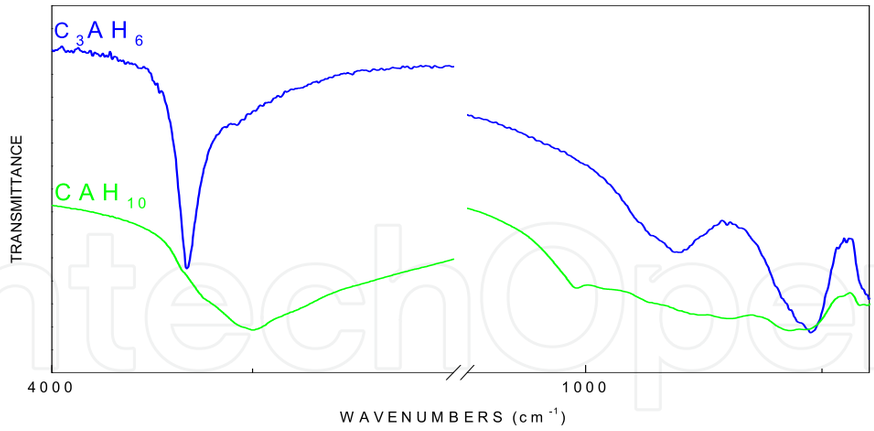


Fig. 12. Infrared spectra of main CAC hydrates, CAH_{10} and C_3AH_6.

area of 3000-3700 cm-1 of the various polymorphs of the aluminium hydroxide (Fig. 13), the spectroscopy of the calcium aluminate cement does not specify clearly the difference between the three forms of the $Al(0H)_3$. However and as guidance that can help in the interpretation, the bayerite has a band in 3550 cm^{-1}, a shoulder in 3430 cm^{-1} and one other shoulder in 3660 cm^{-1}; these are not observed in the spectrum of gibbsite. Table 4 shows the bands of greater interest in the three polymorphisms, according to some authors (Fernández, Frederickson, Van der Marel).

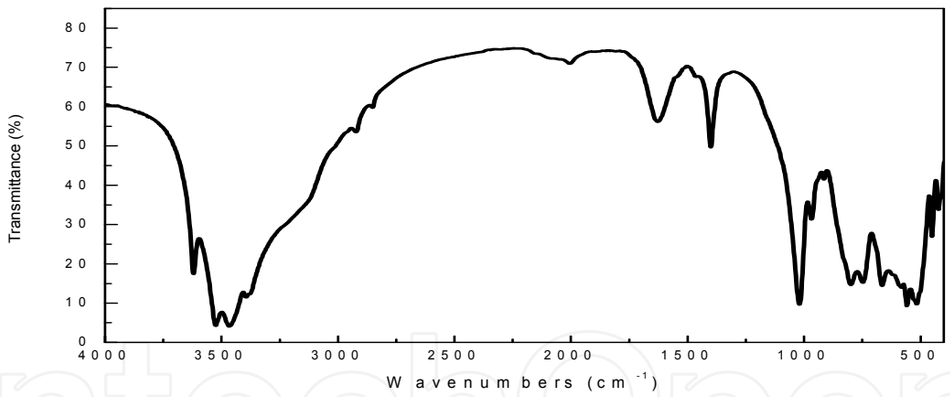


Fig. 13. Aluminium hydroxide, gibbsite, infrared spectra.

	Absorption bands (cm^{-1})	references
Gibbsite	3620, 3524, 3468, 3395 1025, 969	Fernández
Bayerite	3360, 3620, 3540, 3420, 3401, 3454, 3533 1024, 975	Frederickson
Nordstrandite	3660, 3558, 3521, 3490, 3455, 3380, 3360 1060, 1030, 823, 770, 461	Van der Marel

Table 4. Characteristic frequencies of aluminium hydroxides.

4. Carbonated compounds

The infrared spectroscopy is very sensitive to detect the presence of carbonates. The bands more features and more valid for its identification are those indicated in Table 5. The *Calcium carbonate* phases formed after portlandite carbonation, calcite, aragonite or/and vaterite; although vaterite is the least thermodynamically stable of the three crystalline calcium carbonate polymorphs. Indeed, vaterite has been observed following exposure of C-S-H gels to carbon dioxide (accelerated carbonation). The formation of vaterite may occur upon carbonation of pastes with high lime contents, and is favoured by the presence of imperfectly crystalline portlandite. The observed absorptions bands for calcium carbonate phases are due to the planar CO_3^{-2} ion. There are four vibrational modes in the free CO_3^{-2} ion: i) the symmetric stretching, $\nu_1[CO_3]$; ii) the out-of-plane bend, ν_2 $[CO_3]$; iii) the asymmetric stretch, $\upsilon_3[CO_3]$; and iv) the split in-plane bending vibrations $\nu_4[CO_3]$; and Ca-O lattice vibrations. Depending on the calcium carbonate polymorph the vibration of the bands appears at different wavenumber. Figure 14 shows the spectra of calcite, vaterite and aragonite.

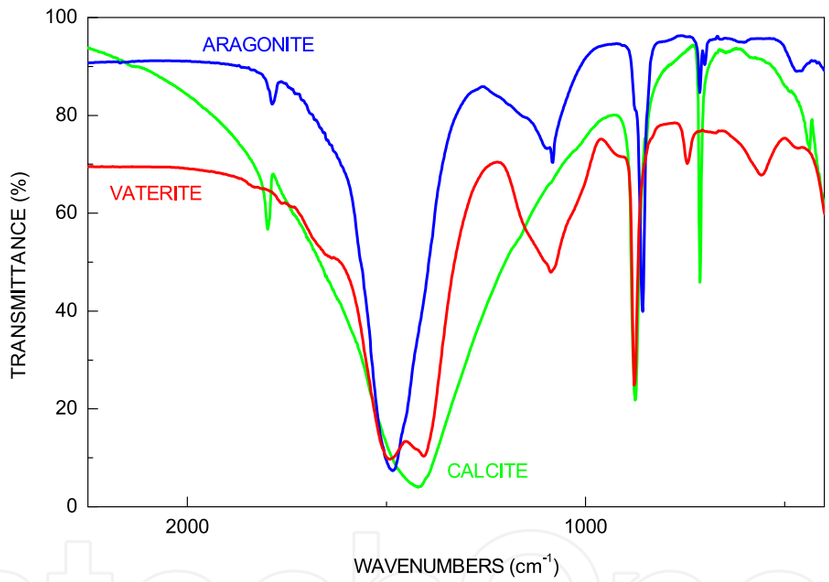


Fig. 14. Infrared spectra of calcite, vaterite and aragonite.

	calcite	vaterite	aragonite
ν_1	1063	1085	
ν_3	1420	1482	1492-1404
ν_4	875, 848	856	877
ν_2	712	713, 700	744

Table 5. Calcium carbonate polymorphs infrared bands

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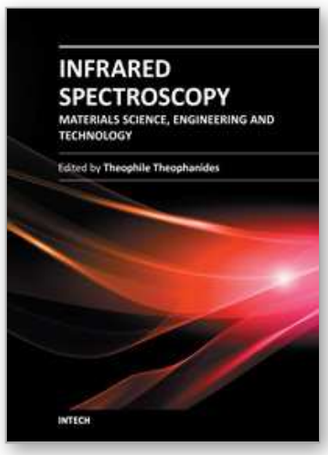
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