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A short hydrogen bond investigation by polarized Raman spectra of Co^{2+} and Zn^{2+} salts of pyromellitic acid

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Abstract

Cobalt and zinc salts of 1,2,4,5-benzenetetracarboxylic acid (pyromellitic acid), $[C_6H_2(COO)_4H_4]$, have been synthesized and investigate by polarized Raman spectroscopy. These compounds present short intramolecular hydrogen bonds (SHB) between adjacent carboxyl groups. Raman spectra indicate the presence of this interaction in both salts. Three specific vibrational of SHB modes have been investigated: O–H–O symmetric [ν_{sym}(OHO)] and asymmetric [ν_{asym}(OHO)] stretching modes and O–H stretching mode [ν(O–H)], which they were observed around 300, 850 and 2500 cm^{-1}, respectively. In crystallographic point of view, the cobalt salt presents a symmetric SHB while the zinc salt presents an asymmetric SHB. In cobalt salt all three vibrational modes of O–H–O groups in polarized Raman spectra occur in A_g orientation although in zinc salts two of them are observed in A_g orientation and one in B_g. Spectra analysis indicate that ν_{sym}(OHO) mode is observed as A_g to cobalt salt and B_g to zinc salt. This mode occurs in a crowed spectral region and its identification was made by deconvolution techniques. Comparing spectra of the two salts, it is observed a small difference in relative intensity and wavenumber shift of ν_{sym}(OHO) (deviance of 43 cm^{-1}) and ν(OH) (deviance of 21 cm^{-1}) modes due probably to differences in O···O distance between salts and in orientation of pyromellitate anion in unit cell. The ν_{asym}(OHO) mode does not present significant wavenumber shift due difference in SHB. The ν(OH) band presents a great potential for hydrogen bond studies due to the fact that in its vibrational region (around 2500 cm^{-1}) it is not observed other vibrational modes of these compounds.

Keywords: Short hydrogen bond; Raman spectroscopy; Pyromellitate salts

1. Introduction

Polycarboxylic acids are important systems to hydrogen bonding studies [1–10]. Anions of these acids can form intramolecular hydrogen bonds (HB), as can be seen in Fig. 1. In particular, the divalent anion of 1,2,4,5-benzenetetracarboxylic acid (pyromellitic acid) has adjacent carboxyl groups that favour intramolecular short hydrogen bond (SHB) formation. Several X-ray structural studies of its derivative compounds show SHB interaction, mainly in divalent anion [11–16].

In crystallographic point of view, hydrogen bonds can be classified as symmetric and asymmetric one. Symmetric HB is the interaction observed between atoms that are symmetrically related, where H atom is located in a special position (two-fold axe, inversion center or mirror plane). In asymmetric HB the atoms are symmetrically independent. Crystal structure of acid salts of pyromellitic acid shows the predominance of asymmetric intramolecular SHB interaction, therefore, these compounds become very interesting systems for charge density studies [17].

Vibrational studies of HB are concentrated in infrared spectroscopy (IR), mainly in O–H stretching mode [ν(OH)]. However, at ν(OH) region, very broad bands appear in IR spectra of hydrate compounds, complicating the assignment of other HB modes. As vibrational modes of water molecules are, in general, very weak in Raman spectra, they do not perturb the analysis of HB bonds in hydrate polycarboxylic compounds [18]. Reid [19] interpreted the changes in the infrared spectra by making a semiempirical treatment of the hydrogen bond based on the Lippincott and Schroeder potential [20]. This treatment used a harmonic oscillator approximation to calculate the O···O stretching frequency with respect to the O···O equilibrium distance. For a short O···O distance (<2.5 Å), a frequency around

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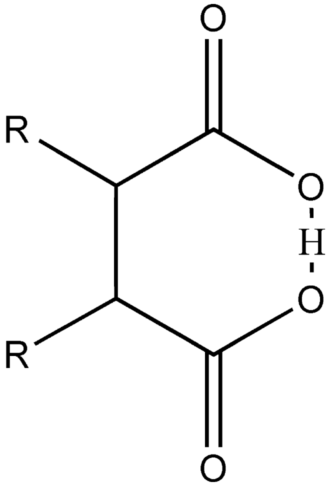

Fig. 1. Representation of short intramolecular hydrogen bond in policarboxylic acids.

$850\,\mathrm{cm}^{-1}$ was found. Miller at al. [21] studied the O···H···O hydrogen bond in $CsH(CF_3CO_2)_2$ and $KH(CF_3CO_2)_2$, that show very short O···O distances. Using Raman spectroscopy, they assigned the O···H···O mode at 798 and $792\,\mathrm{cm}^{-1}$ for Cs and K salts, respectively. Hadzi et al. [2] have also discussed the Raman and infrared spectra of several $MH(CX_3COO)_2$ species and assigned values of 720 and $320\,\mathrm{cm}^{-1}$ for the ν_{asym}(OHO) and ν_{sym}(OHO) bands, respectively. In recent years, some studies of polarized vibrational spectra of compounds presenting HB have been reported [22–25]. In these works the focus of HB investigation was on the ABC band structures [26] and they have investigated the transition dipole moment orientation of HB modes, mainly for ν(OH) and OH deformations. The ABC band structures are related to Fermi resonance between the fundamentals ν(OH) modes of HB and overtones of the bending modes [27]. Spectra of a hydrogen-bonding system show broader, more intense and shifted bands than non-hydrogen-bonding systems [28]. The shift of frequency of ν(OH) is correlated to O···O bond distances [29]. For SHB, this mode occurs in the region of $2000–2500\,\mathrm{cm}^{-1}$. However, for medium and weak HB this mode is found in the region of $3500–3000\,\mathrm{cm}^{-1}$ [29].

In the present work, the stretching modes of O–H–O groups of the SHB interaction have been investigated by polarized Raman spectroscopy using single crystals of hexaaquacobalt(II) dihydrogen 1,2,4,5-benzenetetracarboxylate [CoH_2Bt] and hexaaquazinc(II) dihydrogen 1,2,4,5-benzenetetracarboxylate [ZnH_2Bt]. Powder Raman spectra of these compounds and their deuterated analogues were analyzed by our group [18,30]. The three main short hydrogen bond modes were observed around 300, 850 and $2500\,\mathrm{cm}^{-1}$ assigned to the following SHB stretching modes, ν_{sym}(OHO), ν_{asym}(OHO) and ν(OH) respectively. The wavenumbers of SHB bands obtained from Raman powder data are similar in both salts, even though the different symmetries of SHB observed in crystalline structures. Polarized Raman spectra allow a better assignment of the SHB vibrational bands and can be an interesting tool in its spectral differentiation.

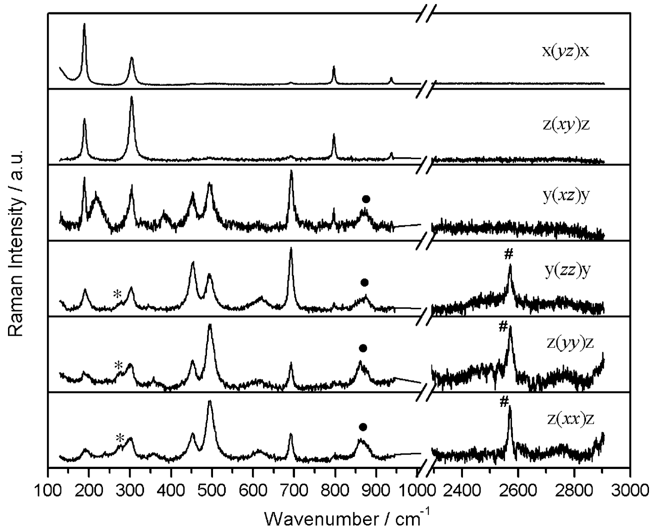

Fig. 2. Raman spectra of A_g and B_g symmetry orientations of CoH_2Bt. The symbol * refers to ν_{sym}(OHO), ● to ν_{asym}(OHO), and # to ν(OH).

2. Experimental

CoH_2Bt and ZnH_2Bt single crystals were obtained by slowly evaporation at room temperature from aqueous solution of cobalt/zinc(II) nitrate hexahydrate (Aldrich 23,037-5, 99%/22,873-7, 98%) and pyromellitic acid (Aldrich B400-7, 96%). Single crystals were oriented by X-ray diffraction method. Raman spectra were recorded on microRaman DILOR X-Y in backscattering configuration and triple monochromator equipped with a CCD detector at room temperature. The 514.5 nm line of an argon ion laser was used as exciting radiation. The measurements have been performed at room temperature in

Table 1
Correlation diagram and analysis of the fundamental modes of CoH_2Bt and ZnH_2Bt

C_{2h}	Internal modes						Raman selection rules
	Salt		H_2BT^{2-}		SHB		
	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	
A_g	28	28	15	15	3	2	(*xx*), (*yy*), (*zz*), (*xz*)
B_g	26	28	15	15	0	1	(*xy*), (*zy*)
A_u	26	27	14	15	2	2	Inactive
B_u	31	28	15	15	1	1	Inactive

SHB: short hydrogen bond modes.

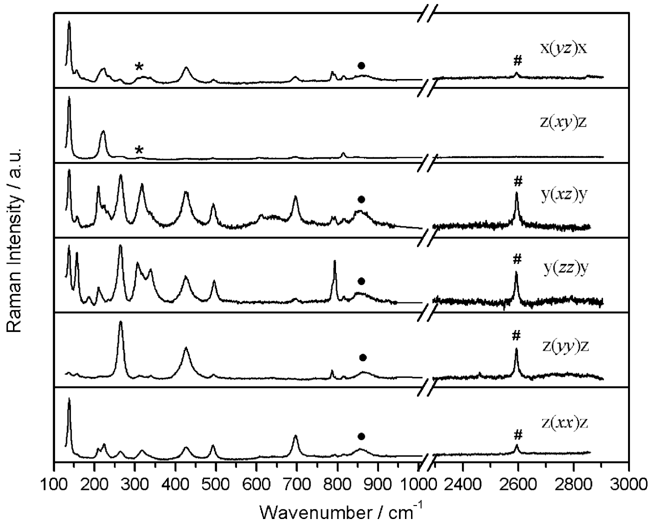

Fig. 3. Raman spectra of A_g and B_g symmetry orientations of ZnH_2Bt. The symbols are defined as Fig. 2.

the region 150–950 and 2300–2900 cm^{-1} region for scattering geometry *z*(*xx*)*z*, *z*(*yy*)*z*, *y*(*zz*)*y*, *y*(*xz*)*y*, *z*(*xy*)*z* and *x*(*yz*)*x* that correspond to A_g (the first four) and B_g (the last two) symmetries. The *x*, *y* and *z* orthogonal coordinate system was chosen in a manner that the *y*-axis were parallel to *b* crystallographic axis. The dissensions of single crystals are about 2 mm × 5 mm × 2 mm for CoH_2BT (prism form) and 3 mm × 2 mm × 5 mm (hexagonal distorted form) for ZnH_2BT in the *a*, *b*, and *c* axes, respectively. Discussions of vibrational results were made using the factor group analysis of the crystals [31]. The tentative assignments of bands were done by deconvolution techniques and previous *ab initio* calculations [18,30].

3. Results and discussion

Polarized Raman spectra for *z*(*xx*)*z*, *z*(*yy*)*z*, *y*(*zz*)*y*, *y*(*xz*)*y*, and *z*(*xy*)*z* and *x*(*yz*)*x* scattering geometry of CoH_2BT and ZnH_2BT are shown in Figs. 2 and 3, respectively. Single crystal X-ray diffraction data show that CoH_2Bt [11] and ZnH_2Bt [16] are ionic, meaning that in both cases the metal is coordinated to water molecules only. They crystallize in monoclinic system, *P*2/*m* and *C*2/*c* space groups, respectively. These two space groups are correlated to C^1_{2h} and C^6_{2h} symmetry group, respectively. Factor group analyses of CoH_2Bt and ZnH_2Bt crystals show 1 1 1 normal modes of vibration (excluding the acoustical modes), where 51 from cation ($[M(H_2O)_6]^{2+}$) and 60 from anion (H_2Bt^{2-}). In CoH_2Bt these modes are distributed in $\Gamma = 28A_g+26B_g+26A_u+31B_u$, and for ZnH_2Bt in $\Gamma = 28A_g+28B_g+27A_u+28B_u$. In this group there are four symmetry types: A_g and B_g (Raman active) and A_u and B_u (IR active). The A_g symmetry is observed in *z*(*xx*)*z*, *z*(*yy*)*z*, *y*(*zz*)*y* and *y*(*xz*)*y* orientations, while B_g symmetry is observed at *z*(*xy*)*z* and *x*(*yz*)*x* orientations. Table 1 displays the classification and selection rules for fundamental modes of the salts. Selected Raman frequencies of cobalt and zinc salts in powder and in crystal with different orientations are listed in Table 2. In Table 3 are listed the SHB geometrical parameters of CoH_2Bt and ZnH_2Bt.

Table 2
Raman wavenumbers (cm^{-1}) and tentative assignment of CoH_2Bt and ZnH_2Bt crystals

z(*xx*)*z*		*z*(*yy*)*z*		*y*(*zz*)*y*		*z*(*xz*)*z*		*z*(*xy*)*z*		*x*(*yz*)*x*		Powder [18,30]		Tentative assignment
CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	CoH_2Bt	ZnH_2Bt	
	138				137		137		136		138			
					156		157				157			
193	209	191		189	186	189		189		189				
239	224					216			217		220			
	262		265		262		263				264			$\delta(\phi)$
274	317	275		277	322	280	316		316		321	307	336	$\nu_{sym}(OHO)$
300		300		302	307	303		304		304				$\delta(\phi)$
358		356	340	347							338			$\delta(COO)$
						385								
451	425	451	426	452	424	452	425				426	452	424	$\nu(M–O)$
495	492	495	496	495	495	492	493				495	485		$\delta(\phi)$
615	610	619		617	610	612	607		612					$\delta(\phi)$
692	696	692		692	696	693	697	694	697	690	695	692	693	$\delta(C–H)$
799		798	787	797	788	796	787	797		796	793	796	785	$\delta(COO)$
	816		814		816		814		816		813	818		$\delta(CH)$
858	855	852	858	849	857	854	854				856	874	860	$\nu_{asym}(OHO)$
								936	916	938				$\nu(CC)+\delta(CH)$
2571	2594	2573	2593	2571	2593		2592				2592	2577	2407	$\nu(OH)$

(: deformation mode; (): aromatic ring, ν: stretching mode.

Table 3
Geometrical parameters of short hydrogen bond in CoH_2Bt and ZnH_2Bt

Salt	O···O (Å)	O–H/H–O (Å)	O–H–O (°)
CoH_2Bt [11]	2.381(2)	1.211(7)	159(2)
ZnH_2Bt [16]	2.413(2)	1.06(4)/1.36(4)	171(4)

In CoH_2Bt, a mirror plane is perpendicular to intramolecular SHB interaction and the O···O distance is 2.381(2) Å. The H atoms of SHB are located in mirror plane symmetry and this interaction is oriented parallel to *b* crystallographic axis. In ZnH_2Bt the SHB is asymmetric which O···O distance of 2.413(2) Å. These SHB are oriented almost along to *a* crystallographic axis.

3.1. Short hydrogen bond vibrations

To both salts, three SHB fundamental modes present Raman activity. As can be observed in Table 1, in CoH_2Bt it is expected all of them in A_g spectra, although in ZnH_2Bt only two are expected. Semi-empirical calculations indicate that stretching modes of O–H–O groups are related to O···O distances [19]. In systems that show SHB (O···O distance between 2.4 and 2.5 Å) the symmetric [ν_{sym}(OHO)] and asymmetric [ν_{asym}(OHO)] stretching modes are expected at about 300 and 850 cm^{-1}, respectively, and the OH stretching [ν(OH)] at around 2500 cm^{-1}. In powder Raman spectra of cobalt [18] and zinc [30] salts, weak and broad bands were observed in these regions (Table 3).

The best region of hydrogen bond investigation is that related to O–H stretching mode, which is very sensitive to formation of this kind of interaction and it is less influenced by other modes in these compounds. This mode occurs only in A_g orientation at 2572 and 2593 cm^{-1} to CoH_2Bt and ZnH_2Bt, respectively. In cobalt salt, this mode has a smaller wavenumber than zinc salt (21 cm^{-1}). These results probably are more related to difference in O···O distance of SHB than to difference in their crystallographic symmetry. This distance in Co salts (2.381(2) Å) is smaller than that observed in ZnH_2Bt (2.413(2) Å). This band in CoH_2Bt does not present a significant intensification in the different A_g orientations, however in ZnH_2Bt is observed intensification in *z*(*yy*)*z* orientation. This effect could be related to difference of anions orientation in crystal cell. In powder Raman spectra of this compounds, the ν(OH) of medium HB is observed at 3450 and 3271 cm^{-1} in CoH_2Bt and ZnH_2Bt, respectively [18,30].

The ν_{asym}(OHO) was also observed in A_g orientation at 858 and 861 cm^{-1} for CoH_2Bt and ZnH_2Bt, respectively. Similar band was not observed in B_g orientation. No significant wavenumber shift is observed to ν_{asym}(OHO) due to crystallographic difference in SHB. In both compounds this mode presents intensification in some orientations. In CoH_2Bt this band is more intense in *z*(*xx*)*z* and *z*(*yy*)*z*, although in ZnH_2Bt this intensification was just observed in *z*(*yy*)*z*. Similar to ν(OH), this effect can be associated to the different orientation of pyromellitate ion in crystal cells. In cobalt salt the O–H–O groups are parallel to *b* crystallographic axis although in zinc salt is almost perpendicular to the same axis.

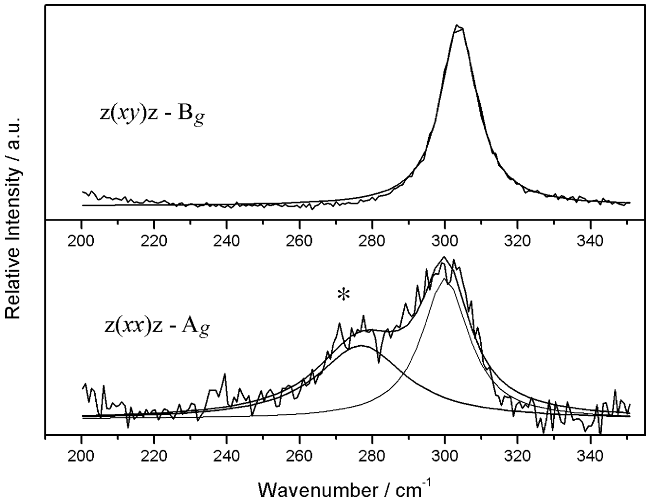

Fig. 4. Raman spectra around ν_{sym}(OHO) band of CoH_2Bt. The symbol * refers to ν_{sym}(OHO).

The vibrational region of ν_{sym}(OHO) (∼300 cm^{-1}) is very complicated to be analyzed due the presence of deformation modes of aromatic ring and water molecules. Due this fact, deconvolution methods were used in single crystal polarized Raman spectra to help the tentative assignment of this mode. These analyses are shown in Figs. 4 and 5 for CoH_2Bt and ZnH_2Bt, respectively. In CoH_2Bt spectra was identified a band in this region in both symmetry orientation (A_g and B_g). Deconvolution treatment (Fig. 4) shows that in A_g symmetry orientation two bands are present, one at 277 cm^{-1} and another at 300 cm^{-1}. In B_g orientation just one band at 304 cm^{-1} is observed. Crystal data show that in this salt the SHB is symmetric and factor group analysis (Table 1) shows that in cobalt salt all SHB modes are Ag. The band shape of A_g orientation is more similar to that observed in powder spectrum, and due these facts, the weak and broad band observed in A_g orientation at 277 cm^{-1} was identi-

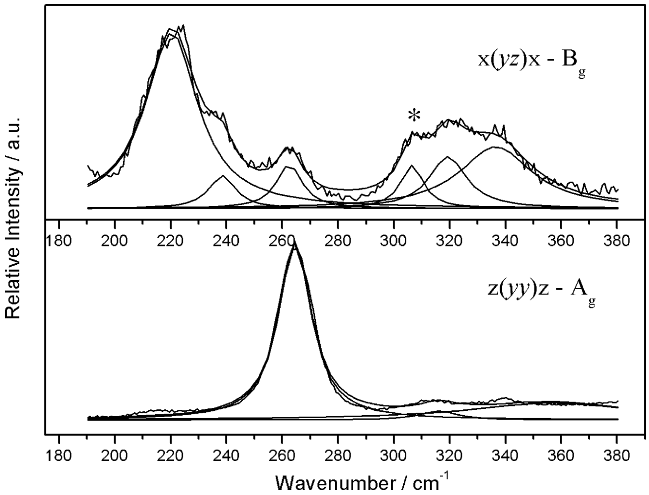

Fig. 5. Raman spectra of ZnH_2Bt in ν_{sym}(OHO) band region. The symbol * refers to ν_{sym}(OHO).

fied as ν_{sym}(OHO) mode. The band observed at 304 cm^{-1} in B_g orientation was tentative assigned as aromatic ring deformation mode [$\delta(\phi)$]. As can be seen in Table 1, one of the SHB modes in ZnH_2Bt is expected in B_g orientation. Two SHB modes were identified in A_g spectra [ν_{asym}(OHO) at 856 cm^{-1} and ν(OH) at 2593 cm^{-1}] and it will be suppose that in this compound the ν_{sym}(OHO) would be observed at B_g spectra. In ZnH_2Bt a weak broad band, similar to cobalt salt, is observed at 320 cm^{-1} in B_g spectra (Fig. 5). A_g spectra [$y(zz)y$ and $x(yz)x$] present bands in the same region but the shape and intensity are different to a typical O–H band.

The ν_{sym}(OHO) mode of cobalt and zinc salts present not only a shift in wavenumber values (around 43 cm^{-1}), like observed in ν_{asym}(OHO), but in its symmetry too. In CoH_2Bt this stretching is A_g and the SHB is symmetric, although in ZnH_2Bt this mode is observed at B_g spectra and the SHB is asymmetric. Similar to that observed in ν(OH), CoH_2Bt spectra present ν_{sym}(OHO) mode in lower wavenumber than in ZnH_2Bt spectra, due mainly to the difference in O···O distance of SHB.

3.2. Other internal vibrations

Some vibrational frequencies and tentative assignments are listed in Table 2. In the vibrational region analyzed (200–1000 cm^{-1}) of cobalt and zinc salts is observed more bands in A_g spectra than in B_g orientations (Figs. 2 and 3). These results indicate that the most deformation modes of aromatic ring [$\delta(\phi)$] and carboxyl groups [δ(COO)] reveal A_g symmetry. The bands observed in B_g spectra of cobalt salts are tentative assigned to benzene ring deformation at 304 cm^{-1}, in plane carboxyl group deformation at 796 cm^{-1} and in plane benzene ring deformation at 936 cm^{-1} [32,33]. In B_g spectra of zinc salt were observed bands at 340, 494, 612 and 816 cm^{-1} assigned to in plane carboxyl deformation, benzene ring deformation (two bands) and in plane C–H deformation, respectively.

In CoH_2Bt A_g spectra were observed bands assigned to benzene ring deformation (300, 495 and 615 cm^{-1}), C–H in plane deformation (692 cm^{-1}), carboxyl group deformation (355 and 787 cm^{-1}) and M–O stretching mode (451 cm^{-1}). A_g spectra of ZnH_2Bt present bands at 262, 492 and 610 cm^{-1} assigned to benzene ring deformation, at 696 and 816 cm^{-1} to C–H in plane deformation, at 787 cm^{-1} assigned to carboxyl group deformation and at 492 cm^{-1} to M–O stretching mode.

4. Conclusions

The CoH_2Bt [11] and ZnH_2Bt [16] are ionic and crystallize in monoclinic system, in $P2/m$ and $C2/c$ space groups, respectively. Both space groups are correlated to C_{2h} point group symmetry, which four symmetry types are present: A_g and B_g (Raman active) and A_u and B_u (IR active). In despite of the CoH_2Bt and ZnH_2Bt space groups are correlated to the same point group (C_{2h}) the mainly SHB modes (three stretching modes) have different symmetries. In cobalt compound (symmetric SHB) the three modes are A_g although in zinc salt two are A_g and one is B_g. In both salts the ν_{asym}(OHO) and ν(OH) modes are A_g, however the ν_{sym}(OHO) is A_g in CoH_2Bt and B_g in ZnH_2Bt.

Small differences are observed in relative intensity and wavenumber shift of ν_{sym}(OHO) and ν(OH) modes. Comparing ZnH_2Bt spectra it can be seen a great intensification of SHB bands. The ν_{sym}(OHO) band is more intense in $y(zz)y$ and $y(xz)y$ orientations although ν_{asym}(OHO) and ν(OH) bands are intensified in $z(yy)z$ orientation. On the other hand, in CoH_2Bt spectra only ν(OH) band showed a small intensification in $z(xx)z$ orientation. This difference in intensity could be related to different orientations of pyromellitate anions in crystal cell. Another difference in Raman spectra of these compounds is the shift in wavenumber in ν_{sym}(OHO) and ν(OH) bands. In CoH_2Bt these modes occur in smaller wavenumber (277 and 2572 cm^{-1}) than in ZnH_2Bt (317 and 2593 cm^{-1}). The wavenumber shifts observed to these modes (40 and 21 cm^{-1}, respectively) are significant and suggest that occurs due the difference in O···O distance (2.381(2) Å to CoH_2Bt and 2.413(2) Å to ZnH_2Bt) than to difference of SHB symmetry.

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