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Data Article

Data of infrared vibration spectroscopy of cyclotriphosphates

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ABSTRACT

By taking the IR spectra of several cyclotriphosphates of a resolved structure, has subsequently shown that it is possible to characterize the P_3O_9 ring by its IR spectrum and, in some favorable cases, to make them Predicted symmetry of the cycle by examining the number, profile and position of the observed infrared bands in the symmetric valence vibration of the POP (ν_s POP) groups. He identified criteria for each type of symmetry and discussed, using concrete examples, the limits of the infrared method in determining the symmetry of the cycle (all the possible symmetries that a P_3O_9 cycle can have). Recently, at the Laboratory, studies have been undertaken by A. ABOUIMRANE et al. [1] for the calculation of the normal IR frequencies of the P_3O_9 cycle for the ideal and real symmetries: D_{3h} , C_s and C_3 (Tables 1,2 and 3).

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Specifications Table

Subject area	Chemistry
More specific subject area	Spectroscopy
Type of data	Table
How data was acquired	Infrared and Raman spectroscopy
Data format	analyzed, calculated
Experimental factors	These calculations were conducted using the semi-empirical method, Modified Neglect of Differential Overlap
Experimental features	The calculation of the frequencies was carried out first of all for the highest symmetry that the P_3O_9 cycle can have, that of its molecular group D_{3h} , then it was carried out for lower symmetries.
Data source location	Laboratory of Physical Chemistry of Materials LCPM, Faculty of Sciences Ben M'sik, B.P. 7955. Bd Cdt Driss El Harti. Hassan II University of Casablanca. Morocco
Data accessibility	With this article
Related research article	S. Zerraf, M. Belhabra, A.Kheireddine, R. Lamsatfi, M.Tridane, H. Moutaabbid, B. Baptiste, M. Moutaabbid, and S. Belaouad, Reinvestigation of the crystal structure of barium cesium Cyclotriphosphate dihydrate and vibrational study, Phosphorus Sulfur Silicon Relat Elem., 192, 2017, 1286–1293 [2].

Value of the data

- These data are useful for researchers working on spectral spectroscopy of cyclotriphosphates.
- These data can be used to develop the spectral vibration of the cyclotriphosphate because they contain experimental vibrations and calculated vibrations.
- The added value of these data is in the theoretical and experimental study of infrared and Raman frequencies in the different symmetric cyclotriphosphate, which contributes to the development of research in the spectral field.

1. Data

The dataset shows how to determine different types of spectral vibration, as shown in Fig. 1. Tables 1–3 refer to the frequencies to be calculated using different simulations in infrared and Raman spectroscopy. The comparison between the experimental and calculated vibration frequencies shows a total of 30 normal vibration patterns were identified for the isolated symmetry cycle D_{3h} . The normal frequency calculation of the P_3O_9 cycle makes it possible to calculate the values of the internal vector component corresponding to the displacement of each atom of the cycle (see Fig. 2–4).

For each frequency, the percentage of participation of the vibrations that contributed to it was specified. The percentages of the two groups, P-Oi-P and POe2 of the ring, were calculated from the

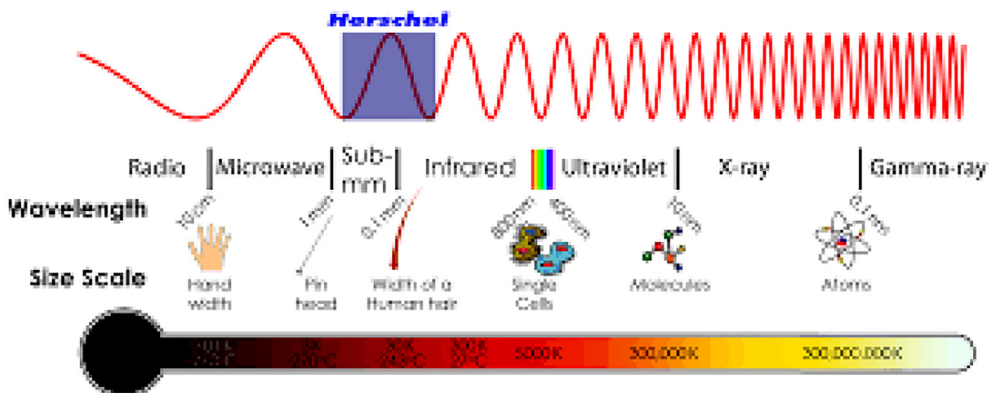


Fig. 1. Infrared radiation.

Table 1
Calculated IR frequencies for symmetry D_{3h} .

ν_{cal} (cm^{-1})	(%) de participation	Mode	ν_{cal} (cm^{-1})	(%) de participation	Mode
1288	ν_{as} PO ₂ [99]	A'' ₂	420	γ_w PO ₂ [78]	A' ₂
{ 1272	ν'_{as} PO ₂ [100]	E''	{ 418	γ' POP [59] γ_T PO ₂ [41]	E''
1272			418		
{ 1225	ν'_{as} POP [98] ν_s PO ₂ [2]	E'	{ 302	δ PO ₂ [98]	A' ₁
1225			299		
1169	ν_s PO ₂ [100]	A' ₁	{ 299	δ' POP[40] γ_w PO ₂ [60]	E'
{ 1108	ν'_{as} POP [18] ν_s PO ₂ [82]	E'	281		
1108			281		
1059	ν_{as} POP [100]	A' ₂	{ 257	δ' POP [26] γ_w PO ₂ [74]	E'
{ 781	ν'_s POP [73] δ PO ₂ [27]	E'	256		
781			214		
671	ν_s POP [52] δ PO ₂ [48]	A' ₁	49	γ POP [27] γ_R PO ₂ [73]	A'' ₂
559	δ POP «δcycle»[78] δ PO ₂ [22]	A' ₁	{ 36	γ' POP [33] γ_R PO ₂ [68]	E''
511	γ POP [60] γ_R PO ₂ [40]	A'' ₂	34		
{ 437	δ' POP [21] δ PO ₂ [79]	E'	{ 437		
437			437		

Table 2
Calculated IR frequencies for symmetry C_s.

ν_{cal} (cm^{-1})	(%) de participation	mode	ν_{cal} (cm^{-1})	(%) de participation	mode
1299	ν_{as} PO ₂ [98]	A'	427	δ' POP [24]	δ' PO ₂ [76] A''
1280	ν_{as} PO ₂ [100]	A'	420	δ' POP [44]	δ' PO ₂ [56] A'
1280	ν_{as} PO ₂ [100]	A''	415	γ_w PO ₂ [77]	A''
1200	ν_{as} POP [98] ν_s PO ₂ [2]	A''	305	δ POP [11]	δ PO ₂ [89] A'
1188	ν_a POP [96] ν_s (PO ₂) [4]	A'	303	γ' POP [16]	γ_T PO ₂ [84] A''
1155	ν_s PO ₂ [98]	A'	297	δ' POP [30]	γ_w PO ₂ [70] A'
1099	ν_{as} POP [18] ν_s PO ₂ [82]	A''	287	γ' POP [14]	γ_T PO ₂ [86] A'
1095	ν_{as} POP [21] ν_s PO ₂ [79]	A'	268	δ' POP [33]	γ_w PO ₂ [67] A''
1032	ν_{as} POP [94]	A''	255	δ' POP [24]	γ_w PO ₂ [76] A''
794	ν_s POP [77] δ PO ₂ [23]	A''	252	δ' POP [20]	γ_w PO ₂ [80] A'
792	ν_s POP [76] δ PO ₂ [24]	A'	214	γ_T PO ₂ [99]	A''
698	ν_s POP [64] δ PO ₂ [36]	A'	104	δ' POP [12]	γ_R PO ₂ [78] A'
563	δ POP [71] δ PO ₂ [29]	A'	89	γ' POP [31]	γ_R PO ₂ [69] A''
513	γ POP [63] γ_R PO ₂ [37]	A'	59	γ' POP [31]	γ_R PO ₂ [69] A'
447	γ' POP [62] γ_T PO ₂ [38]	A''			
447	γ' POP [49] γ_T PO ₂ [51]	A'			

successive isotopic substitutions 31P–33P, 16O_i–18O_i and 16O_e–18O_e. It has been assumed that internal oxygens are not involved in PO_e2 movements and that oxygens outside the cycle are not involved in PO_iP movements. The behavior of the eigenvectors, the displacement of the atoms with respect to their equilibrium position, and therefore of the relative movements at each normal frequency, with respect to the elements of symmetry of the group of the isolated P3O9 cycle, makes it possible to specify their symmetry and consequently the normal modes Corresponding. The assignment of the cycle frequencies is made without any a priori hypothesis and without vibrational spectra [1].

These allocations (Tables 1–3) of the frequencies calculated for the corresponding modes for the symmetries D_{3h} , C_s and C₃ respectively were confirmed by the IR and Raman vibrational spectra of the compounds containing the P₃O₉ cycles of symmetry C_s (Table 5). This table shows how the normal modes change from the symmetry D_{3h} to the symmetry C_s of the isolated cycle. It shows the concordance between the values of the calculated frequencies and the experimental frequencies observed. Indeed, the IR spectra (Table 4) and those of Raman microspectrometry (Table 6) confirm the

Table 3
Calculated IR frequencies for symmetry C_3 .

ν_{calc} (cm^{-1})	(%) de participation	Mode	ν_{calc} (cm^{-1})	(%) de participation	Mode
1298	$\nu_{\text{as}} \text{PO}_2$ [98]	A	428	δ' POP [25] δPO_2 [75]	E
{1280 1279}	$\nu_{\text{as}} \text{PO}_2$ [98]	E			
{1182 1180}	$\nu_{\text{as}} \text{POP}$ [93] $\nu_{\text{s}} \text{PO}_2$ [7]	E	303	δPO_2 [98]	A
1159	$\nu_{\text{s}} \text{PO}_2$ [99]	A	{302 301}	γ' POP [8] $\gamma_{\text{T}} \text{PO}_2$ [92]	E
{1100 1098}	$\nu_{\text{as}} \text{POP}$ [25] $\nu_{\text{s}} \text{PO}_2$ [75]	E	{273 273}	δ' POP [49] $\gamma_{\text{W}} \text{PO}_2$ [51]	E
1025	$\nu_{\text{as}} \text{POP}$ [99]	A	{248 248}	δ' POP [15] $\gamma_{\text{W}} \text{PO}_2$ [85]	E
{800 799}	$\nu_{\text{s}} \text{POP}$ [78] δPO_2 [22]	E	216	$\gamma_{\text{T}} \text{PO}_2$ [100]	A
706	$\nu_{\text{s}} \text{POP}$ [68] δPO_2 [32]	A	102	γPOP [23] $\gamma_{\text{R}} \text{PO}_2$ [77]	A
558	δPOP [58] δPO_2 [42]	A	{80 79}	γ' POP [30] $\gamma_{\text{R}} \text{PO}_2$ [70]	E
501	γPOP [72] $\gamma_{\text{R}} \text{PO}_2$ [28]	A			
{461 461}	$\gamma' \text{POP}$ [61] $\gamma_{\text{T}} \text{PO}_2$ [39]	E			

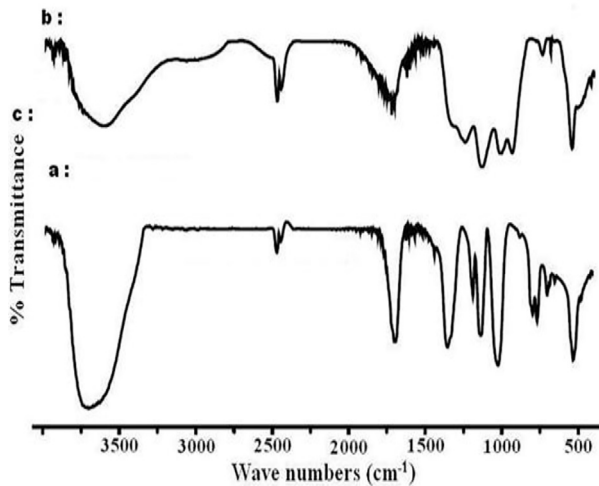


Fig. 2. IR spectra of cyclotriphosphates. (a) $\text{CoK}_4(\text{P}_3\text{O}_9)_2 \cdot 7\text{H}_2\text{O}$, (b) $\text{NiK}_4(\text{P}_3\text{O}_9)_2 \cdot 7\text{H}_2\text{O}$.

proposed assignments of both the valence frequencies and the deformation frequencies of the P_3O_9 cycle.

(Table 7) gives the calculated IR frequencies for the symmetries D_{3h} , C_5 and C_3 and specifies their variations with respect to those calculated for the highest symmetry D_{3h} .

2. Experimental design, materials and methods

These calculations were carried out using the semi-empirical method, Modified Neglect of Differential Overlap (MNDO) [2]. Thus, the calculation made it possible to obtain, for each of the normal

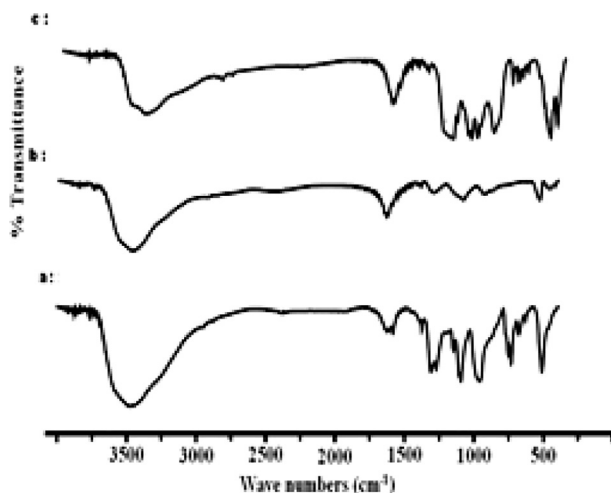


Fig. 3. IR spectra of cyclotriphosphates. (a) $\text{SrNH}_4\text{P}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$, (b) $\text{SrRbP}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$, (c) $\text{SrKP}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$.

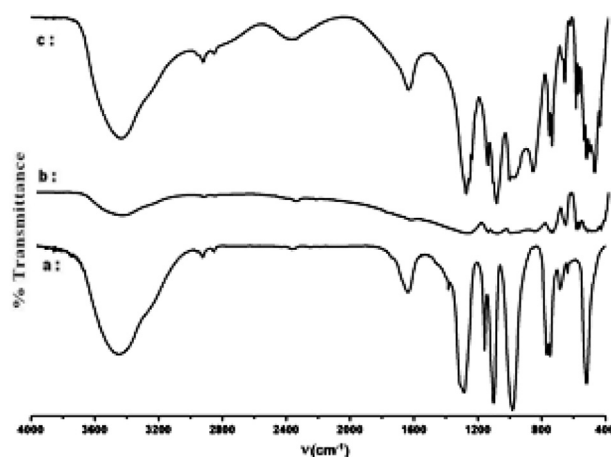


Fig. 4. IR spectra of cyclotriphosphates. (a) $\text{ZnK}_4(\text{P}_3\text{O}_9)_2 \cdot 6\text{H}_2\text{O}$, (b) $\text{ZnRb}_4(\text{P}_3\text{O}_9)_2 \cdot 6\text{H}_2\text{O}$, (c) $\text{NiRb}_4(\text{P}_3\text{O}_9)_2 \cdot 6\text{H}_2\text{O}$.

frequencies of the P_3O_9 cycle, the values of the components of the eigenvectors corresponding to the displacements of each atom of the cycle.

For the calculated normal frequencies of the P_3O_9 cycle, the geometric variations of the elongations and angular deformations of the 12 P_3O_9 ring atoms corresponding to each were calculated. These movements made it possible to attribute the twelve fundamental valence frequencies, for which the variations of distances, P-Oe or P-Oi, are the most important at the 12 highest frequencies. Whereas for the other 18 vibrations of angular deformations the variations of the distances are zero or very small. On the basis of the atomic displacements, the valence frequencies and the deformation frequencies of the P_3O_9 cycle were distinguished and assigned.

Table 4

IR and far IR frequencies (in cm^{-1}) observed in cyclotriphosphates with a P_3O_9 cycle of symmetry C_3 : $\text{SrRbP}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$ (I), $\text{SrNH}_4\text{P}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$ (II), $\text{SrKP}_3\text{O}_9 \cdot 3\text{H}_2\text{O}$ (III), $\text{CoK}_4(\text{P}_3\text{O}_9)_2 \cdot 7\text{H}_2\text{O}$ (IV), $\text{NiK}_4(\text{P}_3\text{O}_9)_2 \cdot 7\text{H}_2\text{O}$ (V), $\text{ZnK}_4(\text{P}_3\text{O}_9)_2 \cdot 6\text{H}_2\text{O}$ (VI), $\text{ZnRb}_4(\text{P}_3\text{O}_9)_2 \cdot 6\text{H}_2\text{O}$ (VII) et $\text{NiRb}_4(\text{P}_3\text{O}_9)_2 \cdot 6\text{H}_2\text{O}$ (VIII).

(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)	(VIII)
1296 (F)	1289 (F)	1306 (F)	1302 (F)	1302 (F)	1284 (F)	1278 (F)	1281 (F)
1255 (F)	1265 (F)	1274 (F)			1255 (F)	1267 (F)	1267 (ép)
	1249(m)						
1203 (f)			1237 (F)	1238 (F)	1196 (f)	1196 (f)	1195 (f)
1157 (F)	1160 (F)	1162 (m)	1155(m)	1155 (m)	1155 (m)	1154 (m)	1159 (m)
1093 (F)	1094 (F)	1122 (F)	1102 (F)	1102 (F)	1096 (F)	1100 (F)	1096 (F)
		1097 (F)		1091 (F)			
1061 (f)	995 (ép)	1009 (F)	1002 (F)	1002 (F)	1031 (F)	1021 (F)	1015 (F)
989 (F)	974 (F)	972 (F)			1014 (F)		
966 (F)							
862 (f)	860 (ép)		861 (f)	849 (f)	879 (f)	881 (f)	923 (ép)
826 (f)							826 (f)
766 (F)	769 (F)	767 (F)	770 (ép)	767 (F)	779 (ép)	08 (m)	743 (F)
721 (f)		735 (F)	744 (F)	738 (F)	744 (F)	741 (F)	
700 (f)	700 (F)	682 (m)	667 (f)	690 (f)		641 (m)	679 (ép)
652 (f)	662 (f)	638 (f)		662 (m)			641 (f)
	651 (m)						
606 (f)							
528 (F)	538 (F)	537 (F)	540 (m)	543 (F)	520 (ép)	548 (ép)	541 (ép)
				537 (ép)			
				529 (ép)			
517 (m)	516 (F)	512 (m)	521 (ép)	514 (F)	514 (F)	514 (F)	504 (F)
		510 (F)	512 (F)		506 (ép)		
498 (f)	457 (m)	452 (m)	493 (ép)	495 (ép)	486 (ép)	464 (m)	464 (m)
457 (f)	387 (f)	384 (m)	469 (m)	471 (ép)	465 (m)	400 (ép)	396 (f)
	374 (f)	366 (F)	412 (f)	450 (ép)	382 (f)	388 (f)	341 (F)
	364 (m)	335 (m)	376 (m)	412 (m)	338 (m)	338 (m)	307 (F)
	336 (m)	323 (m)	354 (f)	375 (F)	329 (ép)	331 (ép)	274 (m)
	322 (m)	310 (m)	336 (m)	326 (ép)	314 (f)	310 (ép)	256 (f)
	312 (F)	283 (F)	323 (m)	321 (F)	301 (m)	300 (m)	235 (m)
	289 (F)	218 (F)	305 (f)	302 (m)	273 (f)	271 (f)	210(F)(Ni ²⁺)
	215 (F)	205 (m)	295 (ép)	288 (f)	236 (m)	236 (m)	179 (f)
	191(F)(Sr ²⁺)	192(F)(Sr ²⁺)	261 (ép)	263 (m)	205 (ép)	183(F)(Zn ²⁺)	150 (F)
	183 (F)	172 (F)	250 (m)	237 (m)	190(F)(Zn ²⁺)	142 (ép)	100 (F)(Rb ⁺)
	161 (F)	125 (F)	229 (f)	215(F)(Ni ²⁺)	161 (m)	127 (F)	95 (F)(Rb ⁺)
	146 (m)	109 (F)(K ⁺)	213(f)(Co ²⁺)	198 (ép)	124 (F)	95 (F)(Rb ⁺)	72 (f)
	117(F)(NH ₄ ⁺)	105 (F)	174 (F)	183 (F)	110 (ép)(K ⁺)	75 (m)	
	82 (m)	77 (F)	154 (F)	157 (F)	92 (ép)	60 (f)	
	71 (F)	65 (f)	139 (m)	152 (F)	74 (f)	55 (m)	
	67 (ép)		130 (ép)	120 (F)(K ⁺)	72 (f)		
	61 (m)		116(m)(K ⁺)	95 (m)	62 (ép)		
			110(m)(K ⁺)	80 (m)			
			93 (m)	69 (m)			
			70 (m)				

Table 5Assignment of the calculated frequencies to the corresponding modes for the Cs symmetry of the P₃O₉ cycle.

Groupe moléculaire D _{3h}			Groupe de site C _s				
v _{cal} (cm ⁻¹)	I _{cal} (Km/mol)	Mode Activité	v _{cal} (cm ⁻¹)	I _{cal} (Km/mol)	NiK ₄ (P ₃ O ₉) ₂ ·7H ₂ O IR	Raman	mode
1287.75	4263.73	A'' ₂ (IR, -)	→ 1298.95	3698.20	1302 (F)	1283 (tf)	A'
{	1271.80	E'' (-, Ra)	→ 1280.48	83.36		1264 (tf)	A'
	1271.79		→ 1280.40	0.45			A''
{	1225.00	E' (IR,Ra)	→ 1200.00	7057.98	1238 (F)		A''
	1224.94		→ 1187.72	7035.81		1236 (f)	A'
{	1168.89	A' ₁ (-, Ra)	→ 1154.85	128.50	1155 (m)	1153 (TF)	A'
	1108.24	E' (IR,Ra)	→ 1098.54	571.79	1102 (F)	1096 (tf)	A''
{	1108.21		→ 1094.95	357.70	1091 (F)	1074(m)	A'
	1059.25	A' ₂ (-, -)	→ 1032.25	2.08	1002 (F)	982 (tf)	A''
{	780.69	E' (IR,Ra)	→ 793.90	1378.24	767 (F)	779 (tf)	A''
	780.68		→ 792.19	1245.65	738 (F)	768 (tf)	A'
{	670.86	A' ₁ (-, Ra)	→ 698.35	185.08	690 (f)	680 (F)	A'
					662 (m)		
	558.95	A' ₁ (-, Ra)	→ 563.09	24.34	543 (F)	540 (m)	A'
					537 (ép)		
					529(ép)		
	511.25	A'' ₂ (IR, -)	→ 513.11	583.14	514 (F)	504 (f)	A'
{	436.70	E' (IR,Ra)	→ 447.29	244.26	495 (ép)	474 (tf)	A''
	436.68		→ 447.13	653.54	471 (ép)		A'
{	420.07	A' ₂ (-, -)	→ 427.38	1215.58			A''
	418.47	E'' (-, Ra)	→ 420.41	580.69	412 (m)	409 (ép)	A'
{	418.41		→ 414.67	10.38			A''
					375 (F)	393 (f)	
{	301.96	A' ₁ (-, Ra)	→ 304.56	27.13	326 (ép)	327 (f)	A'
	298.71	E' (IR,Ra)	→ 302.94	144.56	321 (F)		A''
{	298.67		→ 296.75	234.03	302 (m)	305 (f)	A'
	280.95	E'' (-, Ra)	→ 286.66	11.24	288 (f)	294 (ép)	A'
{	280.92		→ 268.26	54.81	263 (m)		A''
	256.50	E' (IR,Ra)	→ 254.58	18.43			A''
{	256.49		→ 251.50	32.24	237 (m)	237 (tf)	A'
	214.13	A'' ₁ (-, -)	→ 214.46	0.00	215 (F)		A''
					198 (ép)		
					183 (F)		
					157 (F)	162 (tf)	
					152 (F)		
						142 (tf)	
					120 (F) (K ⁻)		
					95 (m)		
					80 (m)		
					69 (m)		
{	49.08	A'' ₂ (IR, -)	→ 104.21	15.37			A'
	35.78		→ 88.62	0.23			A''
{	34.40	E'' (-, Ra)	→ 58.58	2.91			A'

Table 6Distribution of the normal modes of vibration of the $P_3O_9^{3-}$ ion in the isolated state of the various possible symmetries.

Groupe Moléculaire	$\Gamma_{vib}(P_3O_9^{3-})$	Activité		Coïncidence
		IR	Ra	
D_{3h}	$4 A'_1 (Ra) + A''_2 + 2 A'_2 + 3 A''_2 (IR) + 6 E' (IR, Ra) + 4 E'' (Ra)$	9	14	6
$*C_{3h}$	$6 A' (Ra) + 6 E' (IR, Ra) + 4 A'' + 4 E'' (Ra)$	10	16	6
$\sim C_{3v}$	$7 A_1 (IR, Ra) + 3 A_2 + 10 E (IR, Ra)$	17	17	7
$*C_{3v}$	$10 A_1 (IR, Ra) + 5 A_2 (Ra) + 7 B_1 (IR, Ra) + 8 B_2 (IR, Ra)$	25	30	25
$*C_3$	$10 A (IR, Ra) + 10 E (IR, Ra)$	20	20	20
$*C_2$	$15 A (IR, Ra) + 15 B (IR, Ra)$	30	30	30
$*C_s$	$17 A' (IR, Ra) + 13 A'' (IR, Ra)$	30	30	30
C_s	$16 A' (IR, Ra) + 14 A'' (IR, Ra)$	30	30	30
$*C_1$	$30 A (IR, Ra)$	30	30	30

*: The currently known symmetries of the P_3O_9 ring.**Table 7**Calculated IR frequencies for the symmetries C_3 and C_s and their variations with respect to those of the symmetry D_{3h} .

Groupe moléculaire D_{3h}		Groupe de site C_3			Groupe de site C_s			Mouvement
ν (cm^{-1})	I	ν (cm^{-1})	I(Km/mol)	$\Delta\nu$ (cm^{-1})	ν (cm^{-1})	I(Km/mol)	$\Delta\nu$ (cm^{-1})	
1287.75	4263.73	1297.99	3606.74	10.24	1298.95	3698.20	11.20	$\nu_{as} PO_2$
1271.80	0.00	1279.64	369.47	7.84	1280.48	83.36	8.68	$\nu_{as} PO_2$
1271.79	0.00	1278.64	367.77	6.85	1280.40	0.45	8.61	
1225.00	7713.49	1182.29	6964.05	<u>-42.71</u>	1200.00	7057.98	<u>-25.00</u>	$\nu_{as} POP$
1224.94	7714.09	1179.72	6956.35	<u>-45.22</u>	1187.72	7035.81	<u>-37.22</u>	
1168.89	0.00	1158.95	257.24	-9.89	1154.85	128.50	-14.04	$\nu_s PO_2$
1108.24	451.50	1100.13	229.46	-8.11	1098.54	571.79	-9.7	$\nu_s PO_2$
1108.21	451.18	1098.32	180.93	-9.89	1094.95	357.70	-13.26	
1059.25	0.00	1024.87	9.41	<u>-34.38</u>	1032.25	2.08	<u>-27</u>	$\nu_{as} POP$
780.69	1415.41	799.69	1255.39	<u>19</u>	793.90	1378.24	13.21	$\nu_s POP$
780.68	1414.34	799.40	1251.00	<u>18.72</u>	792.19	1245.65	11.51	
670.86	0.00	705.64	392.15	<u>34.78</u>	698.35	185.08	<u>27.49</u>	$\nu_s POP$
558.95	0.01	557.53	15.73	-1.42	563.09	24.34	-4.14	δ POP
511.25	885.11	500.82	508.40	-10.43	513.11	583.14	1.86	γ POP
436.70	1305.47	427.69	1004.20	-9.01	427.38	1215.58	-9.32	$\delta' PO_2$
436.68	1305.75	427.69	1004.28	-8.99	420.41	580.69	<u>-16.27</u>	
420.07	0.00	413.98	6.51	-6.09	414.67	10.38	-5.4	$\gamma_w PO_2$
418.47	0.01	461.40	229.77	<u>42.93</u>	447.29	244.26	<u>28.82</u>	$\gamma' POP$
418.41	0.26	460.80	224.71	<u>42.39</u>	447.13	653.54	<u>28.72</u>	
301.96	0.01	303.22	92.63	1.26	304.56	27.13	2.6	δPO_2
298.71	219.76	273.47	102.39	<u>-25.24</u>	296.75	234.03	-1.96	$\delta' POP$
298.67	219.66	272.80	102.78	<u>-25.87</u>	268.26	54.81	<u>-30.41</u>	
280.95	0.04	301.54	130.03	<u>20.59</u>	302.94	144.56	<u>21.99</u>	$\gamma'_T PO_2$
280.92	0.04	301.28	127.68	<u>20.36</u>	286.66	11.24	5.74	
256.50	6.45	248.35	4.94	-8.15	254.58	18.43	-1.92	$\gamma'_w PO_2$
256.49	6.43	247.67	5.63	-8.82	251.50	32.24	-4.99	
214.13	0	216.07	1.94	1.94	214.46	0.00	0.33	$\gamma_T PO_2$
49.08	17.99	102.15	16.62	<u>53.07</u>	104.21	15.37	<u>55.13</u>	$\gamma_R PO_2$
35.78	0.00	80.06	1.51	<u>44.28</u>	88.62	0.23	<u>52.84</u>	$\gamma'_R PO_2$
34.40	0.01	78.96	1.47	<u>44.56</u>	58.58	2.91	<u>24.18</u>	

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