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 P3O9 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 (vs 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 P3O9 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 P3O9 cycle for the ideal and real symmetries: D3h, Cs and C3 (Tables 1, 2 and 3).

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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 D3h. The normal frequency calculation of the P3O9 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, POi-P and POe2 of the ring, were calculated from the

![Infrared radiation](image)

Fig. 1. Infrared radiation.
successive isotopic substitutions $^{31}\text{P} - 33\text{P}, 16\text{O} - 18\text{O}$ and $16\text{O} - 18\text{O}$. It has been assumed that internal oxygens are not involved in PO$e_2$ movements and that oxygens outside the cycle are not involved in PO$i_2$ 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 P$_3$O$_9$ 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 $D_{3h}$, $C_3$ and $C_3$ respectively were confirmed by the IR and Raman vibrational spectra of the compounds containing the P$_3$O$_9$ 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 1
Calculated IR frequencies for symmetry $D_{3h}$.

| $\nu_{cal}$ (cm$^{-1}$) | (%) de participation | Mode | $\nu_{cal}$ (cm$^{-1}$) | (%) de participation | Mode |
|-------------------------|----------------------|------|-------------------------|----------------------|------|
| 1288 $\nu_{as}$ PO$_2$ [99] | A'' | 420 $\gamma_w$ PO$_2$ [78] | A' |
| 1272 $\nu_{as}$ PO$_2$ [100] | E'' | 418 $\gamma'$ POP [59] $\gamma_i$ PO$_2$ [41] | E'' |
| 1225 $\nu^{as}$ POP [98] $\nu_{i}$ PO$_2$ [2] | E' | 302 $\delta$ PO$_2$ [98] | A' |
| 1169 $\nu_{i}$ PO$_2$ [100] | A' | 299 $\delta'$ POP [40] $\gamma_w$ PO$_2$ [60] | E' |
| 1108 $\nu^{as}$ POP [18] $\nu_{i}$ PO$_2$ [82] | E' | 281 | |
| 1059 $\nu_{as}$ POP [100] | A'' | 257 $\delta'$ PO [26] $\gamma_w$ PO$_2$ [74] | E' |
| 781 $\nu^{as}$ POP [73] $\delta$ PO$_2$ [27] | E' | 256 | |
| 671 $\nu_{as}$ POP [52] $\delta$ PO$_2$ [48] | A' | 214 $\gamma_i$ PO$_2$ [100] | A'' |
| 559 $\delta$ POP «(cycle)» [78] $\delta$ PO$_2$ [22] | A' | 49 $\gamma'$ POP [27] $\gamma_w$ PO$_2$ [73] | A'' |
| 511 $\gamma$ POP [60] $\gamma'$ PO$_2$ [40] | A' | 36 | |
| 437 $\delta'$ POP [21] $\delta$ PO$_2$ [79] | E' | 34 $\gamma'$ POP [33] $\gamma_w$ PO$_2$ [68] | E'' |

### Table 2
Calculated IR frequencies for symmetry $C_s$.

| $\nu_{cal}$ (cm$^{-1}$) | (%) de participation | Mode | $\nu_{cal}$ (cm$^{-1}$) | (%) de participation | Mode |
|-------------------------|----------------------|------|-------------------------|----------------------|------|
| 1299 $\nu_{as}$ PO$_2$ [98] | A' | 427 $\delta'$ POP [24] $\delta$ PO$_2$ [76] | A' |
| 1280 $\nu_{as}$ PO$_2$ [100] | A' | 420 $\delta'$ POP [44] $\delta$ PO$_2$ [56] | A' |
| 1280 $\nu_{as}$ PO$_2$ [100] | A' | 415 $\gamma_w$ PO$_2$ [77] | A' |
| 1200 $\nu_{as}$ POP [98] $\nu_{i}$ PO$_2$ [2] | A' | 305 $\delta$ POP [11] $\delta$ PO$_2$ [89] | A' |
| 1188 $\nu_{i}$ POP [96] $\nu_{i}(PO_2)$ [4] | A' | 303 $\gamma'$ POP [16] $\gamma_w$ PO$_2$ [84] | A' |
| 1155 $\nu_{as}$ PO$_2$ [98] | A' | 297 $\delta'$ POP [30] $\gamma_w$ PO$_2$ [70] | A' |
| 1099 $\nu_{as}$ POP [18] $\nu_{i}$ PO$_2$ [82] | A' | 287 $\gamma'$ POP [14] $\gamma_w$ PO$_2$ [86] | A' |
| 1095 $\nu_{as}$ POP [21] $\nu_{i}$ PO$_2$ [79] | A' | 268 $\delta'$ POP [33] $\gamma_w$ PO$_2$ [67] | A' |
| 1032 $\nu_{as}$ POP [94] | A' | 255 $\delta'$ POP [24] $\gamma_w$ PO$_2$ [76] | A' |
| 794 $\nu_{i}$ POP [77] $\delta$ PO$_2$ [23] | A' | 252 $\delta'$ POP [20] $\gamma_w$ PO$_2$ [80] | A' |
| 792 $\nu_{i}$ POP [76] $\delta$ PO$_2$ [24] | A' | 214 $\gamma'_T$ PO$_2$ [99] | A' |
| 698 $\nu_{as}$ PO [64] $\delta$ PO$_2$ [36] | A' | 104 $\gamma'$ POP [22] $\gamma_w$ PO$_2$ [78] | A' |
| 563 $\delta$ POP [71] $\delta$ PO$_2$ [29] | A' | 89 $\gamma'$ POP [31] $\gamma_w$ PO$_2$ [69] | A' |
| 513 $\gamma$ POP [63] $\gamma_w$ PO$_2$ [37] | A' | 59 $\gamma'$ POP [31] $\gamma_w$ PO$_2$ [69] | A' |
| 447 $\gamma'$ POP [62] $\gamma'_T$ PO$_2$ [38] | A' | 36 $\gamma'$ POP [33] $\gamma_w$ PO$_2$ [68] | E'' |
| 447 $\gamma'$ POP [49] $\gamma'_T$ PO$_2$ [51] | A' | 34 $\gamma'$ POP [33] $\gamma_w$ PO$_2$ [68] | E'' |
proposed assignments of both the valence frequencies and the deformation frequencies of the P₃O₉ cycle.

(Table 7) gives the calculated IR frequencies for the symmetries D₃h, Cₛ and C₃ and specifies their variations with respect to those calculated for the highest symmetry D₃h.

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
frequencies of the P$_3$O$_9$ 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$_3$O$_9$ cycle, the geometric variations of the elongations and angular deformations of the 12 P$_3$O$_9$ 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$_3$O$_9$ cycle were distinguished and assigned.

![Fig. 3. IR spectra of cyclotriphosphates. (a) SrNH$_4$P$_3$O$_9$.3H$_2$O, (b) SrRpP$_3$O$_9$.3H$_2$O, (c) SrKP$_3$O$_9$.3H$_2$O.](image1)

![Fig. 4. IR spectra of cyclotriphosphates. (a) ZnK$_4$(P$_3$O$_9$)$_2$.6H$_2$O, (b) ZnRb$_4$(P$_3$O$_9$)$_2$.6H$_2$O, (c) NiRb$_4$(P$_3$O$_9$)$_2$.6H$_2$O.](image2)
Table 4
IR and far IR frequencies (in cm\(^{-1}\)) observed in cyclotriphosphates with a P\(_3\)O\(_9\) cycle of symmetry C\(_s\): SrRb\(_2\)PO\(_3\)\(_2\)H\(_2\)O (I), SrNH\(_4\)PO\(_3\)\(_2\)H\(_2\)O (II), SrKP\(_3\)O\(_9\) (III), CoK\(_4\)(P\(_3\)O\(_9\))\(_2\)\(_2\)\(_2\)H\(_2\)O (IV), NiK\(_4\)(P\(_3\)O\(_9\))\(_2\)\(_2\)\(_2\)\(_2\)H\(_2\)O (V), ZnK\(_4\)(P3O9)\(_2\)\(_2\)\(_2\)H\(_2\)O (VI), ZnRb\(_4\)(P3O9)\(_2\)\(_2\)\(_2\)H\(_2\)O (VII) et NiRb\(_4\)(P3O9)\(_2\)\(_2\)\(_2\)H\(_2\)O (VIII).

| (I)  | (II) | (III) | (IV)  | (V)  | (VI) | (VII) | (VIII) |
|------|------|-------|-------|------|------|-------|--------|
| 1296 (F) | 1289 (F) | 1306 (F) | 1302 (F) | 1284 (F) | 1278 (F) | 1281 (F) | 1249 (m) |
| 1203 (f) | 1197 (F) | 1180 (m) | 1194 (m) | 1188 (m) | 1182 (m) | 1185 (m) | 1188 (m) |
| 1157 (F) | 1122 (F) | 1107 (F) | 1102 (F) | 1096 (F) | 1100 (F) | 1096 (F) | 1097 (F) |
| 1061 (f) | 995 (ép) | 1009 (F) | 1002 (F) | 1031 (F) | 1014 (F) | 1015 (F) | 1016 (F) |
| 989 (F) | 974 (F) | 972 (F) | 970 (F) | 970 (F) | 970 (F) | 970 (F) | 970 (F) |
| 862 (F) | 860 (ép) | 866 (F) | 870 (F) | 879 (F) | 881 (F) | 923 (ép) | 926 (F) |
| 766 (F) | 769 (F) | 767 (F) | 770 (F) | 779 (ép) | 789 (m) | 743 (F) | 754 (F) |
| 700 (F) | 700 (F) | 682 (m) | 667 (F) | 690 (F) | 641 (m) | 679 (ép) | 681 (F) |
| 652 (f) | 662 (F) | 638 (F) | 662 (m) | 662 (m) | 662 (m) | 662 (m) | 662 (m) |
| 606 (F) | 538 (F) | 537 (F) | 540 (m) | 543 (F) | 537 (ép) | 529 (ép) | 540 (F) |
| 517 (m) | 516 (F) | 512 (m) | 521 (ép) | 514 (F) | 514 (F) | 514 (F) | 504 (F) |
| 498 (f) | 457 (m) | 452 (m) | 493 (ép) | 495 (ép) | 486 (ép) | 464 (m) | 464 (m) |
| 374 (f) | 374 (F) | 384 (m) | 469 (m) | 471 (ép) | 465 (m) | 400 (m) | 396 (F) |
| 364 (m) | 357 (F) | 356 (m) | 376 (m) | 412 (m) | 338 (m) | 338 (m) | 307 (F) |
| 322 (m) | 323 (m) | 354 (F) | 375 (F) | 329 (ép) | 331 (ép) | 274 (m) | 276 (F) |
| 312 (F) | 312 (F) | 310 (m) | 336 (m) | 326 (m) | 314 (F) | 310 (ép) | 256 (F) |
| 289 (F) | 289 (F) | 283 (F) | 323 (m) | 321 (F) | 301 (m) | 300 (m) | 235 (F) |
| 215 (F) | 218 (F) | 205 (m) | 295 (ép) | 288 (F) | 273 (F) | 271 (F) | 210 (F)(Ni\(^{2+}\)) |
| 191 (F)(Sr\(^{2+}\)) | 192 (F)(Sr\(^{2+}\)) | 261 (F) | 263 (m) | 205 (ép) | 183 (F)(Zn\(^{2+}\)) | 150 (F) | 179 (F) |
| 183 (F) | 172 (F) | 250 (m) | 237 (m) | 190 (F)(Zn\(^{2+}\)) | 142 (ép) | 100 (F)(Rb\(^{+}\)) | 95 (F)(Rb\(^{+}\)) |
| 161 (F) | 125 (F) | 229 (f) | 215 (F)(Ni\(^{2+}\)) | 161 (F) | 127 (F) | 95 (F)(Rb\(^{+}\)) | 72 (F) |
| 146 (m) | 109 (F)(K\(^{+}\)) | 213(F)(Co\(^{2+}\)) | 198 (ép) | 124 (F) | 95 (F)(Rb\(^{+}\)) | 72 (F) | 175 (F) |
| 117(F)(NH\(_4\)) | 105 (F) | 174 (F) | 183 (F) | 110 (ép)(K\(^{+}\)) | 75 (m) | 75 (m) | 75 (m) |
| 82 (m) | 77 (F) | 154 (F) | 157 (F) | 92 (ép) | 60 (F) | 60 (F) | 60 (F) |
| 71 (F) | 65 (F) | 139 (m) | 152 (F) | 74 (F) | 55 (F) | 55 (F) | 55 (F) |
| 67 (ép) | 67 (F) | 130 (ép) | 120 (F)(K\(^{+}\)) | 72 (F) | 72 (F) | 72 (F) | 72 (F) |
| 61 (m) | 61 (F) | 116(m)(K\(^{+}\)) | 95 (m) | 62 (ép) | 62 (ép) | 62 (ép) | 62 (ép) |
| 93 (m) | 93 (F) | 69 (m) | 69 (F) | 69 (F) | 69 (F) | 69 (F) | 69 (F) |
Table 5
Assignment 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}) | l_{cal} | Mode | Activité | v_{cal} (cm^{-1}) | l_{cal} | NiK_{2}(P3O9)_{2}·7H_{2}O | Raman | mode |
|---------------------------|----------------------|----------------|----------|-------------------|--------|----------------------------|--------|------|
| 1287.75 | 4263.73 | A'' | (IR, -) | 1298.95 | 3698.20 | 1302 (F) | 1283 (tf) | A' |
| 1271.80 | 0.00 | E'' | (-, Ra) | 1280.48 | 83.36 | 1264 (tf) | A' |
| 1271.79 | 0.00 | E' | (IR,Ra) | 1280.40 | 0.45 | 1238 (F) | A'' |
| 1225.00 | 7713.49 | E' | (IR,Ra) | 1200.00 | 7057.98 | 1236 (F) | 1153 (TF) | A' |
| 1224.94 | 7714.09 | E' | (IR,Ra) | 1187.72 | 7035.81 | 1155 (m) | 1096 (tf) | A'' |
| 1168.89 | 0.00 | A' | (-, Ra) | 1154.85 | 128.50 | 1102 (F) | 1074 (m) | A' |
| 1108.24 | 451.50 | A' | (IR,Ra) | 1098.54 | 571.79 | 1091 (F) | 982 (tf) | A'' |
| 1108.21 | 451.18 | E' | (IR,Ra) | 1094.95 | 357.70 | 1002 (F) | 982 (tf) | A'' |
| 1059.25 | 0.00 | A' | (-, -) | 1032.25 | 2.08 | 849 (f) | 662 (m) | A' |
| 780.69 | 1415.41 | E' | (IR,Ra) | 793.90 | 1378.24 | 767 (F) | 779 (tf) | A'' |
| 780.68 | 1414.34 | A' | (-, Ra) | 792.19 | 1245.65 | 738 (F) | 768 (tf) | A' |
| 670.86 | 0.00 | E' | (IR,Ra) | 698.35 | 185.08 | 690 (f) | 680 (F) | A' |
| 558.95 | 0.01 | A' | (-, Ra) | 563.09 | 24.34 | 543 (F) | 540 (m) | A' |
| 511.25 | 885.11 | A'' | (IR, -) | 513.11 | 583.14 | 514 (F) | 504 (f) | A' |
| 436.70 | 1305.47 | E' | (IR,Ra) | 447.29 | 244.26 | 450 (f) | 474 (tf) | A'' |
| 436.68 | 1305.75 | E' | (IR,Ra) | 447.13 | 653.54 | 537 (ép) | 529 (ép) | A' |
| 420.07 | 0.00 | A' | (-, -) | 427.38 | 1215.58 | 495 (ép) | 471 (ép) | A'' |
| 418.47 | 0.01 | E'' | (-, Ra) | 420.41 | 580.69 | 409 (ép) | 409 (ép) | A'' |
| 418.41 | 0.26 | A' | (-, Ra) | 414.67 | 10.38 | 412 (m) | 393 (f) | A''' |
| 301.96 | 0.01 | A' | (-, Ra) | 304.56 | 27.13 | 375 (F) | 370 (m) | A' |
| 298.71 | 219.76 | E' | (IR,Ra) | 302.94 | 144.56 | 326 (ép) | 327 (f) | A' |
| 298.67 | 219.66 | E' | (IR,Ra) | 296.75 | 234.03 | 321 (F) | 305 (f) | A'' |
| 280.95 | 0.04 | E'' | (-, Ra) | 286.66 | 11.24 | 288 (F) | 294 (ép) | A' |
| 280.92 | 0.04 | E' | (IR,Ra) | 268.26 | 54.81 | 263 (m) | 263 (m) | A'' |
| 256.50 | 6.45 | E' | (IR,Ra) | 254.58 | 18.43 | 120 (F) | 95 (m) | A' |
| 256.49 | 6.43 | E' | (IR,Ra) | 251.50 | 32.24 | 158 (F) | 80 (m) | A' |
| 214.13 | 0 | A'' | (-, -) | 214.46 | 0.00 | 198 (F) | 198 (F) | A'' |
| 49.08 | 17.99 | A'' | (IR, -) | 104.21 | 15.37 | 162 (tf) | 162 (tf) | A' |
| 35.78 | 0.00 | E'' | (-, Ra) | 88.62 | 0.23 | 152 (F) | 142 (tf) | A'' |
| 34.40 | 0.01 | E'' | (-, Ra) | 58.58 | 2.91 | 120 (F) | 95 (m) | A' |
Table 6
Distribution of the normal modes of vibration of the P₃O₉³⁻ ion in the isolated state of the various possible symmetries.

| Moléculaire | Γ’vib (P₃O₉³⁻) | Activité | Coincidence |
|-------------|-----------------|----------|-------------|
| D₃h         | 4 A’₁ (Ra) + A’₂ + 2 A’₂ + 3 A”₂ (IR) + 6 E’ (IR, Ra) + 4 E” (Ra) | 9        | 14          | 6           |
| C₃h         | 6 A’ (Ra) + 6 E’ (IR, Ra) + 4 A” + 4 E” (Ra) | 10       | 16          | 6           |
| C₃v         | 7 A₁ (IR, Ra) + 3 A₂ + 10 E (IR, Ra) | 17       | 17          | 7           |
| C₂v         | 10 A₁ (IR, Ra) + 5 A₂ (Ra) + 7 B₁ (IR, Ra) + 8 B₂ (IR, Ra) | 25       | 30          | 25          |
| C₂          | 10 A (IR, Ra) + 10 E (IR, Ra) | 20       | 20          | 20          |
| C₂          | 15 A (IR, Ra) + 15 B (IR, Ra) | 30       | 30          | 30          |
| C₂          | 17 A’ (IR, Ra) + 13 A” (IR, Ra) | 30       | 30          | 30          |
| C₂          | 16 A’ (IR, Ra) + 14 A” (IR, Ra) | 30       | 30          | 30          |
| C₂          | 30 A (IR, Ra) | 30       | 30          | 30          |

*: The currently known symmetries of the P₃O₉ ring.

Table 7
Calculated IR frequencies for the symmetries C₃ and Cₛ and their variations with respect to those of the symmetry D₃h.

| Groupe moléculaire D₃h | Groupe de site C₃ | Groupe de site Cₛ | Mouvement |
|------------------------|-------------------|-------------------|-----------|
| ν (cm⁻¹) | I | ν (cm⁻¹) | I(K/mol) | Δν (cm⁻¹) | ν (cm⁻¹) | I(K/mol) | Δν (cm⁻¹) |
| 1287.75 | 4263.73 | 1297.99 | 3606.74 | 10.24 | 1298.95 | 3698.20 | 11.20 | ν₂₉ PO₂ |
| 1271.80 | 1279.64 | 369.47 | 7.84 | 1280.48 | 83.36 | 8.68 | ν₉ PO₂ |
| 1271.79 | 1278.64 | 367.77 | 6.85 | 1280.40 | 0.45 | 8.61 | ν₇ POP |
| 1225.00 | 1182.29 | 694.05 | -42.71 | 1200.00 | 7057.98 | 25.00 | ν₆ PO₂ |
| 1224.94 | 1179.72 | 695.35 | -45.22 | 1187.72 | 7035.81 | 37.22 | ν₆ POP |
| 1168.89 | 1158.95 | 257.24 | -9.89 | 1154.85 | 128.50 | -14.04 | ν₅ PO₂ |
| 1108.24 | 1100.13 | 229.46 | -8.11 | 1098.54 | 571.79 | -9.7 | ν₄ PO₂ |
| 1108.21 | 1098.32 | 180.93 | -9.89 | 1094.95 | 357.70 | -13.26 | ν₃ POP |
| 1059.25 | 1024.87 | 9.41 | 34.38 | 1032.25 | 2.08 | -27 | δ POP |
| 780.69 | 1415.41 | 799.69 | 1255.39 | 19 | 793.90 | 1378.24 | 13.21 | γ PO₂ |
| 780.68 | 1414.34 | 799.40 | 1251.00 | 18.72 | 792.19 | 1245.65 | 11.51 | γ₀ PO₂ |
| 670.86 | 0.00 | 705.64 | 392.15 | 34.78 | 698.35 | 185.08 | 27.49 | δ PO₂ |
| 558.95 | 0.01 | 557.53 | 15.73 | 1.42 | 563.09 | 24.34 | -4.14 | ν₂ PO₂ |
| 511.25 | 885.11 | 500.82 | 508.40 | -10.43 | 513.11 | 583.14 | 1.86 | ν₁ POP |
| 436.70 | 1305.47 | 427.69 | 1004.20 | -9.01 | 427.38 | 1215.58 | -9.32 | δPO₂ |
| 436.68 | 1305.75 | 427.69 | 1004.28 | -8.99 | 420.41 | 580.69 | -16.27 | ν₀ PO₂ |
| 420.07 | 413.98 | 6.51 | -6.09 | 414.67 | 10.38 | -5.4 | γ PO₂ |
| 418.47 | 461.40 | 229.77 | 42.93 | 447.29 | 244.26 | 28.82 | γ₀ PO₂ |
| 418.41 | 460.80 | 224.71 | 42.39 | 447.13 | 653.54 | 28.72 | δ PO₂ |
| 301.96 | 303.22 | 92.63 | 1.26 | 304.56 | 27.13 | 2.6 | ν PO₂ |
| 298.71 | 219.76 | 273.47 | 102.39 | -25.24 | 296.75 | 234.03 | -1.96 | δ PO₂ |
| 298.67 | 219.66 | 272.80 | 102.78 | -25.87 | 268.26 | 54.81 | -40.41 | ν₀ PO₂ |
| 280.95 | 0.04 | 301.54 | 130.03 | 20.59 | 302.94 | 144.56 | 41.99 | γ PO₂ |
| 280.92 | 0.04 | 301.28 | 127.68 | 20.36 | 286.66 | 11.24 | 5.74 | γ₀ PO₂ |
| 256.50 | 6.45 | 248.35 | 4.94 | -8.15 | 254.58 | 18.43 | -1.92 | γ’ PO₂ |
| 256.49 | 6.43 | 247.67 | 5.63 | -8.82 | 251.50 | 32.24 | -4.99 | γ₀ PO₂ |
| 214.13 | 0 | 216.07 | 1.94 | 1.94 | 214.46 | 0.00 | 0.33 | γ’ PO₂ |
| 49.08 | 17.99 | 102.15 | 16.62 | 53.07 | 104.21 | 15.37 | 55.13 | γ’’ PO₂ |
| 35.78 | 0.00 | 80.06 | 1.51 | 44.28 | 88.62 | 0.23 | 52.84 | γ’’’ PO₂ |
| 34.40 | 0.01 | 78.96 | 1.47 | 44.56 | 58.58 | 2.91 | 24.18 | γ’’’ PO₂ |
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