***Supporting Information***

**Growth, crystal structure, Hirshfeld surface analysis, DFT studies, physicochemical characterization and cytotoxicity assays of novel organic triphosphate**

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**Table S-1.** Crystal data and refinement of (C10H15N2)2H3P3O10.

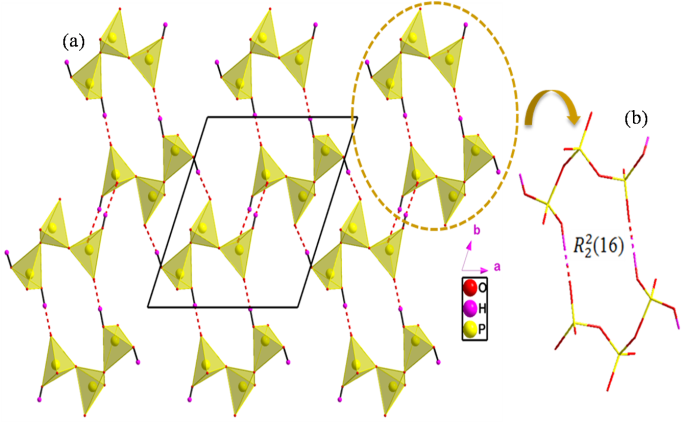
|  |  |
| --- | --- |
| Empirical formula | (C10H15N2)2H3P3O10 |
| Formula weight  Temperature (K)  Wavelength (A ˚ )  Crystal system  Space group  a (Å)  b (Å)  c (Å)  α(°)  β(°)  γ(°)  Volume (Å3)  Z  Dcalc (Mg cm-3)  Absorption coefficient  F (000)  Theta range for data collection  Crystal size (mm3)  Limiting indices  Reflections collected  Reflections observed  Goodness-of-fit on F2  Final R indices  Largest diff. peak and hole (e Å-3) | 582.41 (g.mol-1)  293  0.71073  Triclinic  P  9.511(2)  10.622(2)  13.653(2)  84.58(2)  86.59(2)  68.78(2)  1279.5(4)  2  1.512  0.24 (mm-1)  612  2.06°- 32.78°  0.21 x 0.16 x 0.14  -14<h< 14, -12<k<12, -4<l< 18  8386  6138  1.06  R1 = 0.054 and wR2 = 0.153  0.54 and -0.63 |

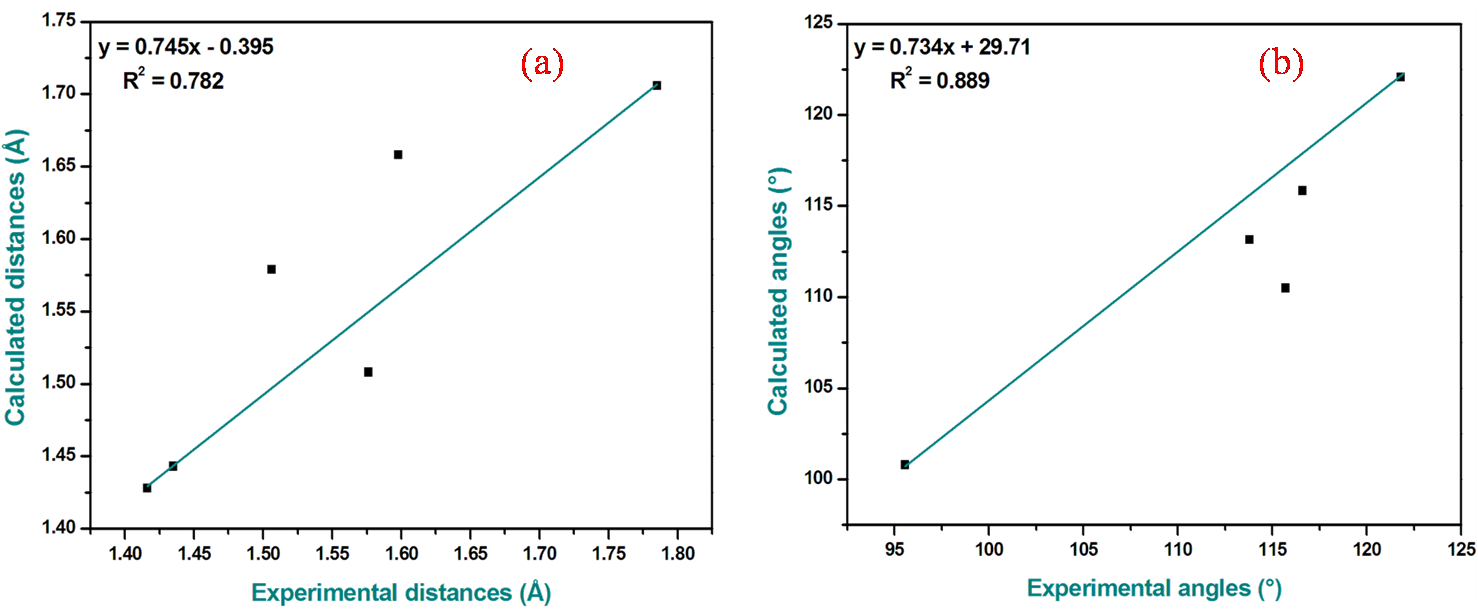
**Table S-2.** Principal intermolecular hydrogen bonding geometry (Å, ˚).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *D-H…A* | *D-H(Å)* | *H...A(Å)* | *D...A(Å)* | *D-H...A(˚)* |
| *O(9)-H(7)…O(8)* | 0.75(5) | 1.89(5) | 2.624(4) | 169(5) |
| *O(1)-H(8)…O(10)* | 0.99(6) | 1.60(6) | 2.557(4) | 162(5) |
| *O(2)-H(9)…O(6)* | 0.89(4) | 1.72(4) | 2.605(3) | 173(5) |
| *N(2)-H(2A)…O(6)* | 0.90 | 2.04 | 2.851(3) | 150 |
| *N(2)-H(2B)…O(7)* | 0.90 | 1.64 | 2.478(3) | 153 |
| *N(4)-H(4A)...O(8)* | 0.90 | 2.22 | 2.991(3) | 143 |
| *N(4)-H(4B)…O(3)* | 0.90 | 1.83 | 2.700(3) | 162 |
| *C(8)-H(8A) ...O(3)* | 0.97 | 2.13 | 2.989(3) | 147 |
| *C(9)-H(9A) ...O(7)* | 0.97 | 2.55 | 3.095(3) | 116 |
| *C(19)-H(19B)...O(10)* | 0.97 | 2.23 | 3.190(4) | 170 |

trip-12.tif

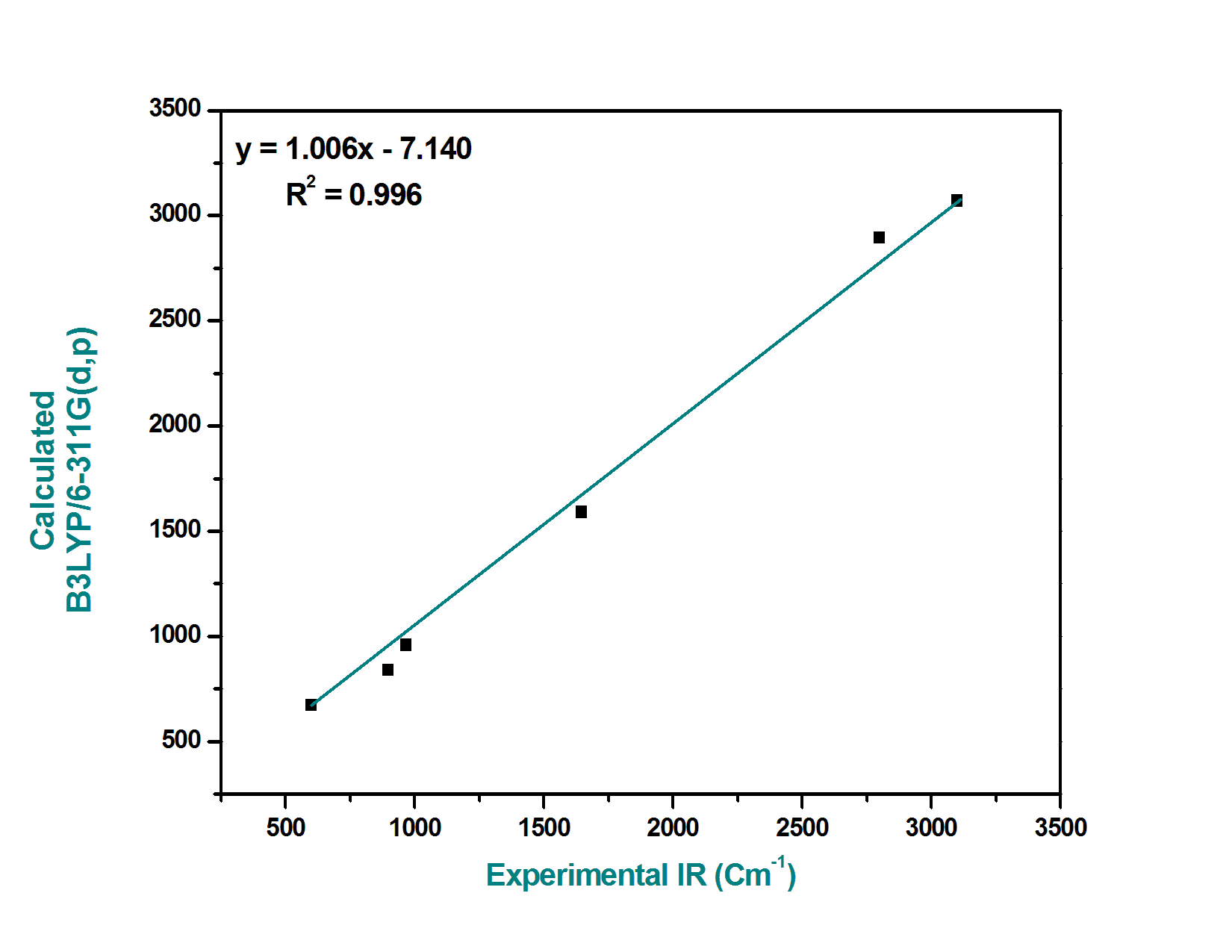
**Figure S-1.** The asymmetric unit of (C10H15N2)2H3P3O10.



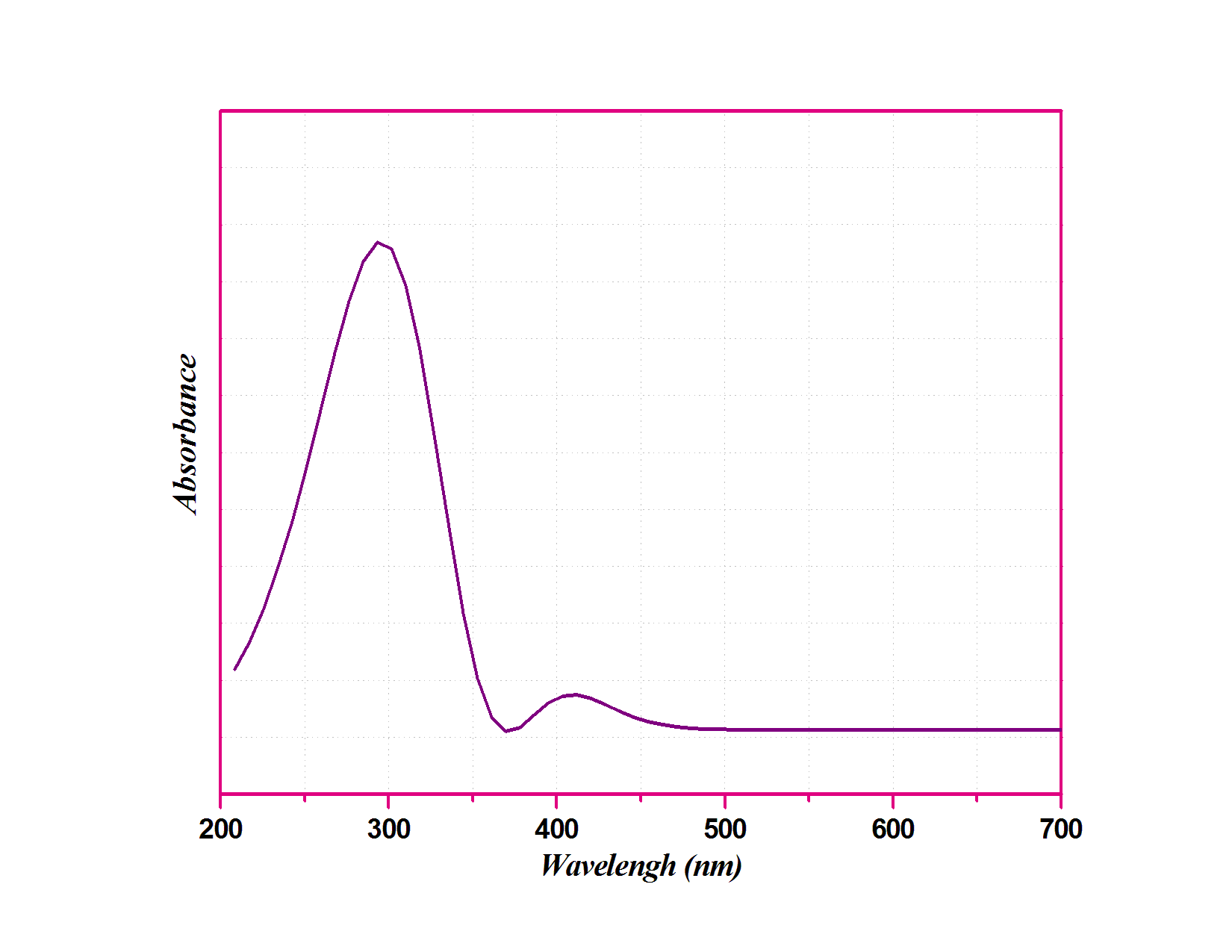
**Figure S-2.** (a) Infinite layers of [H3P3O10]2- viewed along the c axis. (b) Hydrogen bonding sired with dashed lines.

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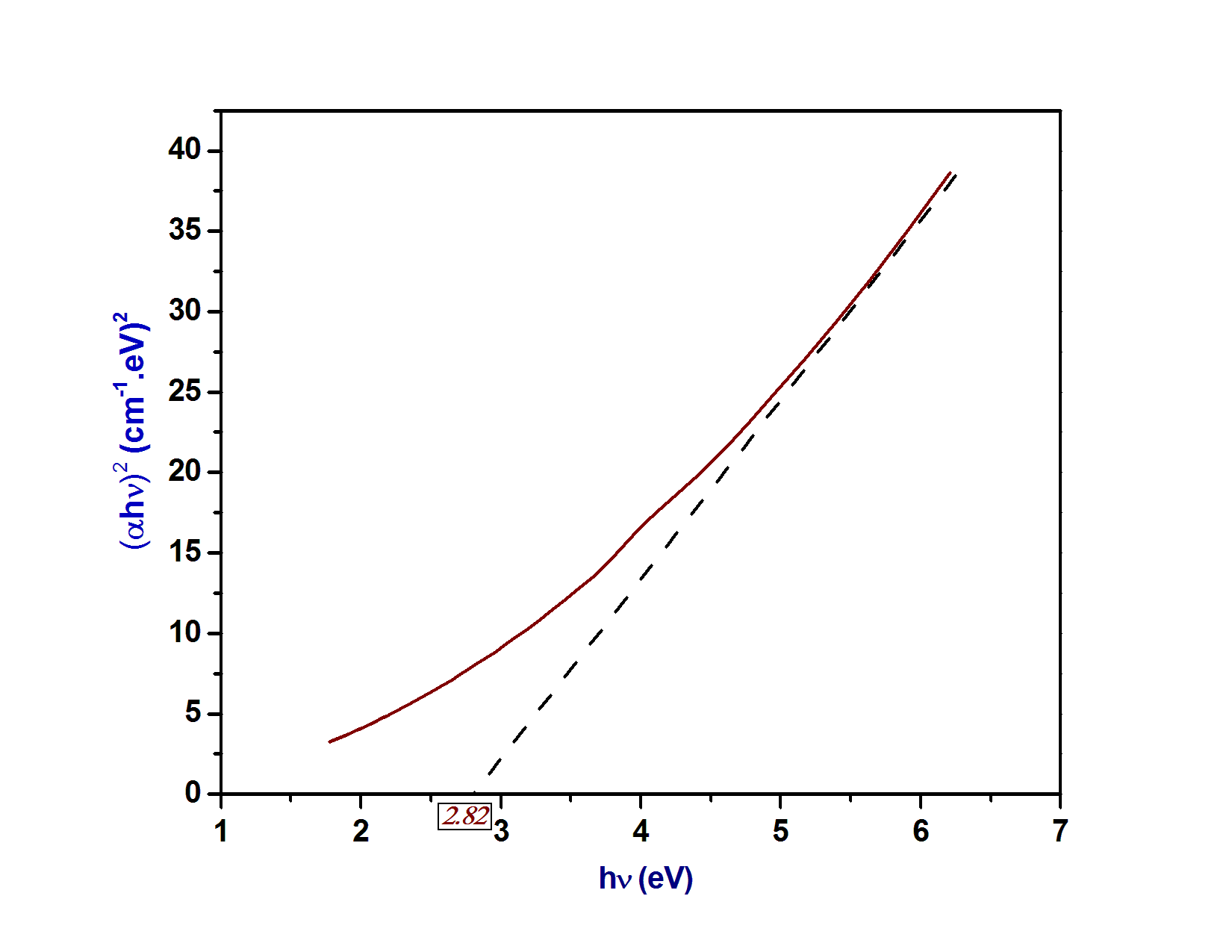
**Figure S-3.** Graphical correlation of theoretical and experimental geometric parameters (a): distances (b): angles.



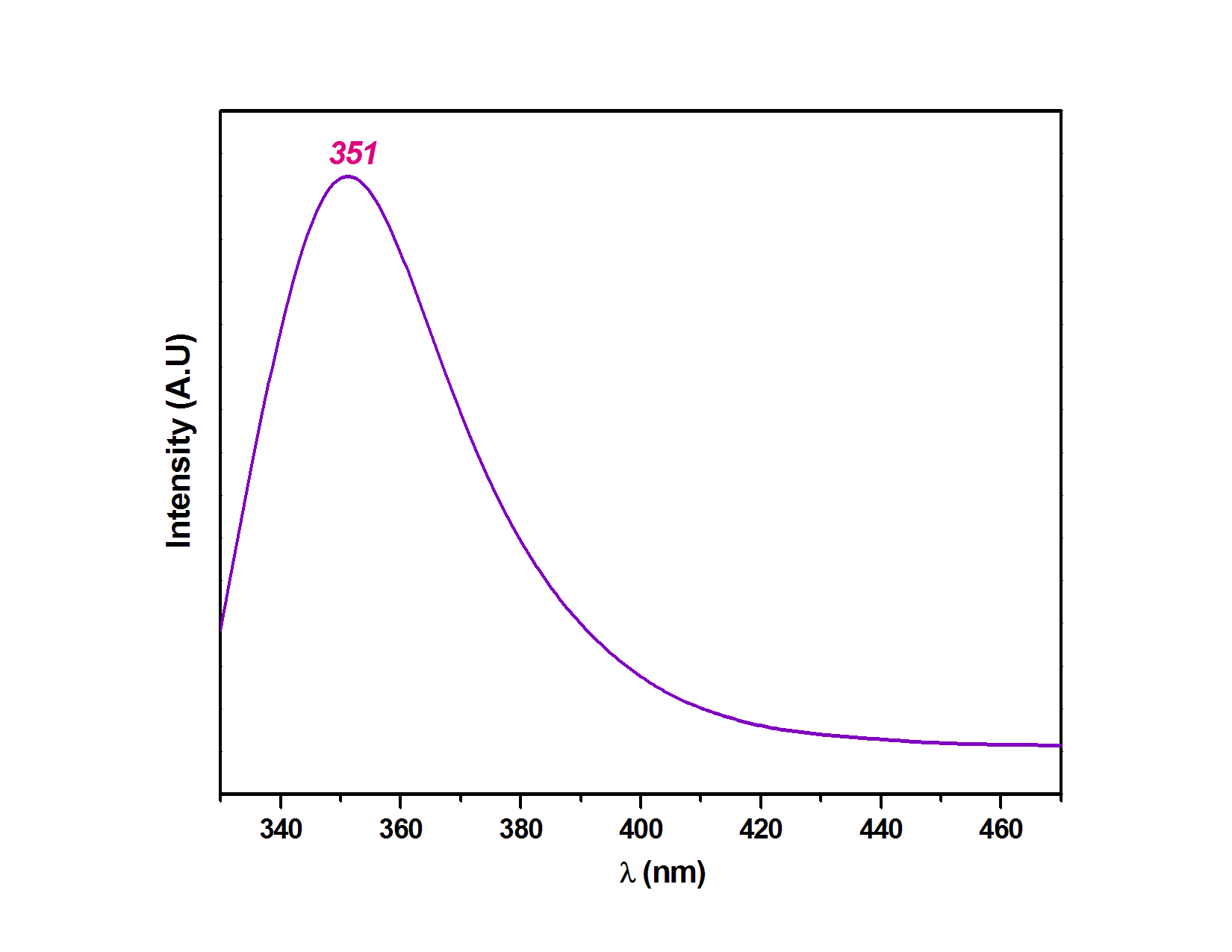
**Figure S-4.** Graphical correlation of theoretical and experimental infrared values.



**Figure S-5.** UV-Vis Spectrum of (C10H15N2)2H3P3O10 in solid state.



**Figure S-6.** Dependence of (αhυ)2 on the photon energy and optical band gap value of (C10H15N2)2H3P3O10.



**Figure S-7.** Solid-state photoluminescence spectrum of (C10H15N2)2H3P3O10.