***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 weightTemperature (K)Wavelength (A ˚ )Crystal systemSpace groupa (Å)b (Å)c (Å)α(°)β(°)γ(°)Volume (Å3)ZDcalc (Mg cm-3)Absorption coefficientF (000)Theta range for data collectionCrystal size (mm3)Limiting indicesReflections collectedReflections observedGoodness-of-fit on F2Final R indicesLargest diff. peak and hole (e Å-3) | 582.41 (g.mol-1)2930.71073TriclinicP$\overbar{1}$9.511(2)10.622(2) 13.653(2)84.58(2)86.59(2)68.78(2)1279.5(4)21.512 0.24 (mm-1)6122.06°- 32.78°0.21 x 0.16 x 0.14-14<h< 14, -12<k<12, -4<l< 18838661381.06R1 = 0.054 and wR2 = 0.1530.54 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 |



**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.