

**POLYMORPHISM  
OF 4,7-DIPHENYL-2,1,3-BENZOTHIADIAZOLE DERIVATIVE CRYSTALS**

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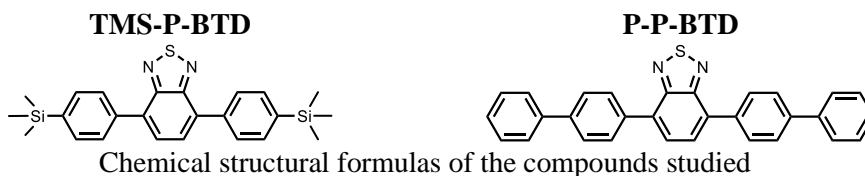
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4,7-Diphenyl-2,1,3-benzothiadiazole (P-BTD) and its derivatives (R-P-BTD) are thermo- and chemically stable luminophores featuring a large Stokes shift and efficient emission in both solutions and crystals. Consequently, they are in demand for a wide range of applications in photonics and electronics [1]. Crystalline materials based on these compounds, both in bulk and thin-film form, are of particular interest. However, according to recent studies, conformational crystal polymorphism is frequently observed in the R-P-BTD family of compounds [1,2], which is of great interest for elucidating structure–property relationships. This work discusses the results of a study on the polymorphism of crystals of R-P-BTD-type compounds bearing trimethylsilyl (TMS-P-BTD) [2] and phenyl (P-P-BTD) terminal substituents (see Figure).



Using single-crystal X-ray diffraction, three polymorphic forms were identified for **TMS-P-BTD**: I – monoclinic (sp. gr.  $P2_1/c$ ,  $Z/Z' = 32/8$ ), II – orthorhombic  $Pnaa$  (sp. gr.  $Pnaa$ ,  $Z/Z' = 12/1.5$ ) and III – triclinic (sp. gr.  $P-1$ ,  $Z/Z' = 8/4$ ) [2]. For **P-P-BTD**, two polymorphic forms were established:  $\alpha$  – triclinic (sp. gr.  $P-1$ ,  $Z/Z' = 2/1$ ;  $a=10.1065(2)$ ,  $b=10.5274(2)$ ,  $c=10.7378(2)$  Å;  $\alpha=91.106(1)^\circ$ ,  $\beta=98.363(1)^\circ$ ,  $\gamma=103.839(1)^\circ$ ) and  $\beta$  – monoclinic (sp. gr.  $C2/c$ ,  $Z/Z' = 16/2$ ;  $a=23.0533(2)$ ,  $b=27.5264(10)$ ,  $c=18.9876(12)$  Å;  $\beta=127.159(1)^\circ$ ). The thermodynamic and kinetic aspects of phase transitions in the studied polymorphic systems are discussed.

1. Echeverri M. et. al. Stimuli-Responsive Benzothiadiazole Derivative as a Dopant for Rewritable Polymer Blends // ACS Appl. Mater. Interfaces. 2020. Vol. 12. P. 10929–10937. <https://doi.org/10.1021/acsami.9b21209>

2. Postnikov V.A. et. al. Conformational Polymorphism of 4,7-Bis(4-(trimethylsilyl)phenyl)- 2,1,3-benzothiadiazole Crystals // Molecules. 2026. Vol. 23. P. 884. <https://doi.org/10.3390/molecules31050884>

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