

عنوان مقاله:

Assessment of explosive properties of new derivative of tetrazine

محل انتشار:

چهارمین کنفرانس بین المللی نوآوری های اخیر در شیمی و مهندسی شیمی (سال: 1396)

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خلاصه مقاله:

This work introduces a novel nitrogen-rich derivatives of tetrazine, i.e. 6,6 -(hexa aza-1,5-diene-1,6-diy)bis(1,2,4,5-tetrazin-3-amine), as high performance and safe energetic compounds. which are evaluated and discussed using some reliable models. The predicted properties are also compared with 2,4,6-trinitrotoluene (TNT) and 1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) as two well-known melt-castable and high performance explosives, respectively. It is shown that one compound can be seen as interesting organic explosives with relatively high performance and low sensitivity, which could be used for important industrial applications. Since some of the new compounds have a relatively good oxygen balance, the calculated specific impulses confirm that these compounds can be considered as suitable oxidizers in solid propellants.

کلمات کلیدی:

Tetrazine, Nitrogen-rich derivatives, TNT, HMX

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