

Abstract Submitted
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On Microscopic Detonation Model LEONID GATILOV, ALEXANDER SELEZENEV, ALEXEI ALEINIKOV, ANZHELA KOMAREVSKAYA, RFNC - VNIIEF — Both computation using the code “Gaussian” with DFT b31yp/6-311++g** method and spectrometry using “Nexus” device have been performed for infrared spectra of HE, including TNT, RDX, HMX and others. The approach proposed in (*A.V.Pozdnyakov, Fizika gorenia i vzryva, 2002, V.38, 3.*) has been basically used to derive correlations between the detonation velocity of individual HE, the effective diameter of HE molecules and the vibrational frequencies of their functional groups. Statistical significance of the resulting correlations has been evaluated by comparing between computed and experimental detonation velocity values. Similarly, detonation velocity computations have been performed for some HE mixtures. The agreement found between the numerical and experimental values of detonation velocity confirms basic concepts of the microscopic detonation model to be developed.

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