Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Influence of nitrogroups positions in molecules of various classes of explosives on results of quantum-chemical calculation of dissociation energy VLADIMIR GOLUBEV, Russian Federal Nuclear Center - VNIIEF — Results of quantum-chemical calculation of dissociation energies of nitrogroups in molecules of various classes of explosives such as aliphatic and aromatic nitrocompounds (C-NO2), aliphatic, heterocyclic (N-NO_2) and aromatic (C-NO_2, N-NO_2) amines, nitrates of spirits (O-NO_2) are presented. Molecules more than thirty explosives, from nitromethane to octogen and PETN are examined. Calculations were carried out with the use of the Gaussian 98 program. The density functional theory (DFT) method with the B3LYP combined functional was applied. Several basic sets of electronic functions, from the widely used polarizing 6-31G(d) basic set to the extremely large multifunctional 6-311++G(3df, 3pd) basic set, were used in calculations. The values of lengths of corresponding bonds and other structural and energetic characteristics of examined molecules are also deduced. Influence of structural isomerism and conformation was considered. The general tendencies of influence of nitrogroups positions in the molecules of explosives on the values of dissociation energy of the bonds were discoverd. For the majority of the considered molecules the certain interrelation of the dissociation energy of the weakest bond and the sensitivity to impact of corresponding explosive was recorded.

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Date submitted: 06 May 2005 Electronic form version 1.4