Abstract Submitted for the SHOCK17 Meeting of The American Physical Society

Ability of thermochemical calculation to treat organic peroxides ANTOINE OSMONT, GRARD BAUDIN, MARC GENETIER, CEA, DAM, GRA-MAT, F-46500 Gramat, France — Since 3 years, the CEA Gramat is developing a new thermochemical code, called SIAME, funded by DGA to help French defense industry at conceiving new explosives compositions. It enables the calculation of CJ detonation and deflagration points and combustion of explosives. The accuracy of the code has been checked on several compositions containing PETN, RDX, HMX, TNT, NTO. The error on the velocity of detonation is 3 %. To enlarge the domain of validity of the code, organic peroxides have been considered. It is known that thermochemical simulation is in failure regarding compounds as simple as hydrogen peroxide. The computed velocity of detonation is 5720 m/s when shock planar impact gives 6150 m/s. The same discrepancy is found for TATP, with a calculated value at 5870 m/s when 5290 has been measured. Detonation velocity of TATP has been measured at two different densities. These velocities agree with other published values. A closer look at the enthalpy of formation of TATP has revealed that it comes from an article of 1932. Ab initio computations have given a totally different value, leading to better agreement with experiment.

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Date submitted: 22 Feb 2017

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