CALCULATION OF DETONATION PROPERTIES OF CHNO EXPLOSIVES USING MOPAC ARCHIVE FILES AS INPUTS

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Recently, application of the Kamlet-Jacobs (K-J) empirical scheme for prediction of detonation properties of energetic materials (EMs) was shown as an effective tool for a fast estimation of a pool of the most promising molecular structures for a high-level treatment [1]. The K-J scheme assumes two quantities, solid state enthalpy of formation ΔH_f and crystal density d_c, are calculated. In this context, semi-empirical method PM7 [2] is very attractive and was recently applied for calculation of the gas-phase ΔH_f of EMs [3].

In the present abstract, we report the development of a new computer code called PM7KJ, which can estimate the solid-state ΔH_f and d_c on the basis of empirical correlations and apply them for calculation of the detonation energy (Q, cal/g), velocity (D, m/s) and pressure (P, GPa). Along with these quantities, the results include the number of moles of detonation gases per 1g of explosive (N) and mean molecular weight of detonation gases ($\bar{M}$). The PM7KJ code is written on the PascalABC.NET programming language and applies the MOPAC2016 [4] archive files (*.arc) as input files for the calculation. Thus, the prediction procedure includes two very fast computations with MOPAC2016 and PM7KJ code runs, normally taking a few minutes to complete. As a result, the PM7KJ code generates a text file, whose heading can be seen in Fig. 1. Along with the detonation properties, the PM7KJ code provides some widely used quantities (in eV) derived from the frontier molecular orbital information. These include, electronegativity (χ), chemical hardness (η) and electrophilicity index (ω).

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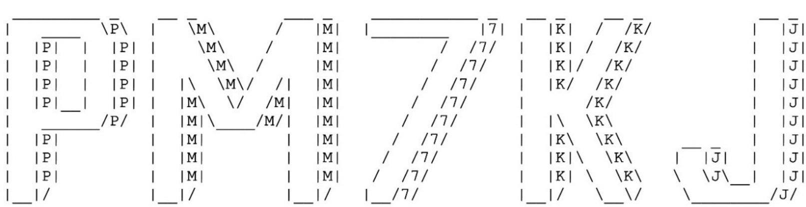

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Fig. 1. Heading fragment of the output file generated by the PM7KJ code

Testing of the developed method in terms of the obtained accuracy of the ΔH_f and d_c values prediction and, subsequently, the accuracy of the obtained K-J results will be done in the corresponding full paper.

References

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[4] Stewart, J. J. P. MOPAC2016, Version: 22.097W; Available at http://openmopac.net/