Synthesis and investigation of the properties of energetic coordination compounds

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Abstract

The subject of the dissertation was to determine the possibility of obtaining new energetic coordination compounds containing aliphatic amine ligands and to examine them from the point of view of safety parameters and the possibility of their practical application as "green" alternatives to pentaerythritol tetranitrate(V) used in detonators. The need to replace this compound, arises from the release during decomposition of toxic gaseous products such as nitrogen oxides, which exhibit toxic effects on the environment. The issue is therefore relevant to the "Green Deal" and to the implementation of waste-free or low-waste processes.

Pentaerythritol tetranitrate(V) is still used today as a high explosive, so other alternative materials are being sought to replace it, while being more environmentally friendly. Potential replacements should meet a number of requirements, such as high thermal and chemical stability, high safety parameters (low friction, impact sensitivity) and a short transition time from burning to detonation.

The physicochemical and energetic properties of were discussed. Particular attention has been paid to compounds in which the central atom consists of Fe, Ni, Cu or Zn atoms, while the ligands are aliphatic amines, heterocyclic compounds (triazoles, tetrazoles, oxadiazoles) and which contain oxidising anions, such as nitrate(V) or chlorate(VII) anion. For most of the compounds discussed, methods of synthesis and potential applications are described. On the basis of the literature review, it was pointed out that the vast majority of the described energetic coordination compounds are compounds containing heterocyclic ligands, while a minority are compounds containing aliphatic ligands. The literature reports indicate that ligands such as 1,2-ethylenediamine and 1,3-diaminopropane, for example, are less used for the synthesis of energetic coordination compounds, hence in this work it was decided to investigate the properties of compounds containing aliphatic ligands.

The experimental part involves the synthesis of energetic coordination compounds containing ligands such as 1,2-ethylenediamine, 1,3-diaminopropane, tris(2-aminoethyl)amine and tris(3-aminopropyl)amine. The choice of the central atoms (Fe, Ni, Cu, Zn) was motivated by their widespread occurrence in the environment (in the form of oxides and salts) and their low toxicity, especially towards lead compounds typically used in detonators. The research carried out includes the determination of the structure of the synthesised compounds, studies of their properties and also describes an attempt to use selected energetic coordination compounds as alternative materials used in detonators. The criterion for the selection of compounds for testing in detonators was low

friction and impact sensitivity as well as high thermal stability. Furthermore, in the context of fuse preparation, the form of the synthesised compound in the form of a fine crystalline powder enabling proper pressing in fuses was important.

Based on the above criteria, compounds were selected for which the maximum shock wave pressure and total explosion energy (Pmax, E) were determined in the underwater explosion test. The results obtained for detonators containing ECCs were related to the results obtained for reference detonators containing 800 mg of pentaerythritol tetranitrate(V) and 300 mg of lead(II) azide. Analysing the parameters describing the detonation characteristics, the nature of the primary shock wave generated by fuses containing chlorate(VII) anion indicated that these compounds detonated, while compounds containing nitrate(V) anion deflagrated.

On the basis of the results obtained, the hypothesis was formulated that, of the energetic coordination compounds synthesised, compounds containing the chlorate(VII) anion, as well as 1,3-diaminopropane as ligand, show the greatest potential for use in detonators as an alternative to the currently used pentaerythritol tetranitrate(V), and could therefore be used as a secondary explosives.