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OPTIMIZATION OF THE ANALYTICAL REAGENT (AR) $Co_3(PO_4)_2 \cdot 8H_2O$ SYNTHESIS CONDITIONS USING THE HARRINGTON'S DESIRABILITY FUNCTION

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Traditional methods for determination of synthesis conditions influencing into chemical compound composition and purity degree are included a lot of experiments needed many time and efforts. Most of it is "passive" because based on the variation of the separate independent variable at conditions, when other ones try to fix. Usually the experiments are multi-factorial that connected with simultaneous optimization of a few parameters.

A convenient way to consolidate optimization criteria which are dissimilar in their nature into one value stands the Harrington's desirability function. It was the result of observations of real solutions experimenters and has nice features such as continuity, monotony and flatness. The mathematical apparatus for transformation of specific parameters in terms of abstract numerical values uses so-called Harrington's logistic function D.

The Box-Wilson experiment design was made for the acceleration and optimization of the analytical reagent (AR) $Co_3(PO_4)_2 \cdot 8H_2O$ synthesis conditions. As optimization criteria of the three callback functions it was used the Harrington's desirability function, which unites the different (of physical content) requirements to the examining object and conditions of its preparation. They are based on the requirements to the chemical of analytical purity – chemically (supra) pure according requirements of State standard of Ukraine (DSTY 2216-93 Reagents and supra pure substances. Designations and methods for determination of purity degrees. Terms and definitions), the efficiency and environmental protection:

1. Molar ratio К=CoO:P_2O_5 must be the closest to 3.00, that responds to its theoretical value in the chemical – factor Y_1;
2. Content of carbonate impurity (expressed as CO_2 (% wt.) must be minimized (for AR chemical – no more 0.1% wt.) – Y_2;
3. Yield of finished product (%) (detected on P_2O_5 content in the remaining stock solution) should be close to 100% – Y_3. Indirectly this factor characterizes the synthesis efficiency and cost of the chemical.

No option separately (Y_1, Y_2, Y_3) can be used as the sole criterion for optimization of the synthesis process, as this would be considered only "one-sided" requirements for the object of study.

The controlling factors influenced into quality of the $Co_3(PO_4)_2 \cdot 8H_2O$ and used for the full-factor Box-Wilson Central Composite Design, are:

1. Temperature –20 - 80 ºС; variable - 30 ºС;
2. H_3PO_4 mass concentration – 10-50 % wt.; variable - 30 % wt.;
3. Duration of the synthesis – 1-3 hours; variable – 1 hour.

It was conducted four parallel experiments for the estimation of the result reproducibility. Conditions of the syntheses responded the centre of the partial replica executing of Box-Wilson Central Composite Design: temperature - 50ºC; H_3PO_4 mass concentration – 30 % wt.; duration of the synthesis – 2 hours. Estimation of the results shown that reproducibility of the obtained data was satisfactory.

On the stage of replica executing of Box-Wilson Central Composite Design (CDD) it was determined the optimal conditions completely corresponded to the specified requirements. Product obtained at the next parameters of synthesis: i) temperature - 80ºC; ii) H_3PO_4 mass concentration – 50 % wt.; iii) duration of the synthesis – 1 hour was characterized practically ideal value of the Harrington's logistic function D= 0,98231.

So, no needed to design the polynomial model and finding local extrema for this multivariable function. The correspondence degree of the chemical composition of isolated salt to the requirements «chemically pure» chemical (AR) was demonstrated by chemical analysis and X-ray method.