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X-RAY DIFFRACTION ANALYSIS OF A DIAMIDOPHOSPHATE-CONTAINING COBALT PHTHALOCYANINE PIGMENT

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Abstract. This study investigates the phase composition and structural features of a diamidophosphate-containing cobalt phthalocyanine pigment by means of X-ray diffraction analysis. The objective was to determine the influence of diamidophosphate modification on the crystalline organization and phase state of the cobalt phthalocyanine framework. Qualitative interpretation of the diffractogram showed that the pigment retained the principal crystalline fragments of the cobalt-centered macrocyclic structure, while the appearance of additional reflections and changes in peak distribution indicated structural reorganization induced by the phosphorus- and nitrogen-containing modifier. The coexistence of sharp diffraction maxima and broadened reflections suggests the formation of a heterogeneous system composed of both ordered crystalline domains and partially disordered regions. Such a structural arrangement indicates that the modification process affected not only the chemical composition of the pigment but also its crystal packing and phase stability. The obtained results confirm that diamidophosphate modification leads to the formation of a hybrid functional pigment with preserved cobalt phthalocyanine core and altered phase characteristics. These features are expected to improve the pigment's

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compatibility with binder systems and enhance its potential for application in high-performance coatings, polymer composites, and other functional materials requiring structural stability and durable color properties.

Keywords: cobalt phthalocyanine pigment, diamidophosphate modification, X-ray diffraction, phase composition, crystal structure, functional pigment, hybrid material, structural reorganization, crystalline domains, polymer-compatible pigment.

Аннотация. В данной работе исследуются фазовый состав и структурные особенности пигмента фталоцианина кобальта, модифицированного диамидофосфатом, с использованием метода рентгенодифракционного анализа (XRD). Целью исследования было определить влияние диамидофосфатной модификации на кристаллическую организацию и фазовое состояние структуры фталоцианина кобальта.Качественная интерпретация дифрактограммы показала, что пигмент сохраняет основные кристаллические фрагменты макроциклической структуры с центром кобальта. В то же время появление дополнительных рефлексов и изменения в распределении пиков свидетельствуют о структурной реорганизации, вызванной модификатором, содержащим фосфор и азот. Совместное наличие чётких дифракционных максимумов и уширенных рефлексов указывает на формирование гетерогенной системы, включающей как упорядоченные кристаллические домены, так и частично разупорядоченные области.Такое структурное строение показывает, что процесс модификации влияет не только на химический состав пигмента, но и на его кристаллическую упаковку и фазовую стабильность. Полученные результаты подтверждают, что диамидофосфатная модификация приводит к образованию гибридного функционального пигмента с сохранённым ядром фталоцианина кобальта и изменёнными фазовыми характеристиками. Эти свойства, как ожидается, улучшат совместимость пигмента со связующими системами и расширят его применение в высокоэффективных покрытиях, полимерных композитах и других функциональных материалах, требующих структурной стабильности и стойкости окраски.

Ключевые слова: пигмент фталоцианина кобальта, диамидофосфатная модификация, рентгенодифракционный анализ, фазовый состав, кристаллическая структура, функциональный пигмент, гибридный материал, структурная реорганизация, кристаллические домены, полимер-совместимый пигмент.

Annotatsiya. Ushbu tadqiqotda diammidofosfat tutuvchi kobalt ftalosiyanin pigmentining fazaviy tarkibi va strukturaviy xususiyatlari rentgen difraksion tahlil (XRD) yordamida o‘rganildi. Tadqiqotning asosiy maqsadi diammidofosfat

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modifikatsiyasining kobalt ftalosiyanin karkasining kristall tuzilishi va fazaviy holatiga ta’sirini aniqlashdan iborat edi.Difraktogrammaning sifat tahlili shuni ko‘rsatdiki, pigment kobalt markazli makrotsiklik tuzilmaning asosiy kristall fragmentlarini saqlab qoladi. Shu bilan birga, qo‘shimcha reflekslarning paydo bo‘lishi va piklar taqsimotidagi o‘zgarishlar fosfor va azot tutuvchi modifikator ta’sirida yuzaga kelgan strukturaviy qayta tashkil topishni ko‘rsatadi. Aniq difraksion maksimumlar va kengaygan reflekslarning birgalikda kuzatilishi tartibli kristall domenlar hamda qisman tartibsiz hududlardan iborat geterogen tizim shakllanganligini anglatadi.Bunday strukturaviy holat modifikatsiya jarayoni nafaqat pigmentning kimyoviy tarkibiga, balki uning kristall qadoqlanishi va fazaviy barqarorligiga ham ta’sir ko‘rsatganini bildiradi. Olingan natijalar diammidofosfat modifikatsiyasi natijasida kobalt ftalosiyanin yadrosi saqlanib qolgan holda, o‘zgargan fazaviy xususiyatlarga ega bo‘lgan gibrid funksional pigment hosil bo‘lishini tasdiqlaydi. Ushbu xususiyatlar pigmentning bog‘lovchi tizimlar bilan mosligini oshirishi hamda uni yuqori samarali qoplamalar, polimer kompozitlar va strukturaviy barqarorlik hamda rangning uzoq muddat saqlanishi talab etiladigan boshqa funksional materiallarda qo‘llash imkoniyatini kengaytirishi kutilmoqda.

Kalit so‘zlar: kobalt ftalosiyanin pigmenti, diammidofosfat modifikatsiyasi, rentgen difraksion tahlil, fazaviy tarkib, kristall tuzilma, funksional pigment, gibrid material, strukturaviy qayta tashkil topish, kristall domenlar, polimer bilan mos pigment.

INTRODUCTION.

Colorants, including dyes and pigments, represent one of the oldest and most widely used classes of functional materials. Since ancient times, they have been employed not only to impart aesthetic value to objects, textiles, architectural elements, and household items, but also to provide protective and functional properties. Over time, the role of colorants has expanded far beyond simple decoration. Today, they are essential components in paints, coatings, plastics, textiles, printing inks, construction materials, ceramics, and various industrial products [1].

Among colorants, pigments occupy a particularly important position because they are generally insoluble in the application medium and provide long-term color stability, opacity, weather resistance, and surface protection. In paint and coating systems, pigments determine not only the color tone and brightness of the final product, but also its covering power, resistance to light, thermal stability, chemical durability, and service life. Therefore, the selection of suitable pigments is one of the key factors in developing high-performance coating materials.

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In recent decades, the demand for paints and coatings has increased significantly due to the rapid development of construction, infrastructure, transport, machinery, household appliances, and industrial manufacturing. This tendency is observed both globally and in our Republic, where large-scale construction projects, modernization of industrial facilities, and expansion of urban infrastructure have created a growing need for durable and cost-effective coating materials. As a result, the demand for high-quality raw materials, especially pigments, has become increasingly important.

The quality of pigments directly affects the technological and operational properties of paint and coating formulations. Pigments with high color intensity allow the production of coatings with lower material consumption, while pigments with improved dispersion stability ensure uniform distribution in the binder matrix and prevent sedimentation during storage. In addition, pigments resistant to ultraviolet radiation, moisture, heat, and aggressive chemical environments contribute to the long-term durability of protective coatings used under outdoor and industrial conditions [2].

Metal phthalocyanine pigments constitute an important class of functional macroheterocyclic compounds characterized by high color strength, pronounced thermal resistance, photochemical stability, and a highly conjugated π-electron system [3,4]. Their practical importance is associated not only with their intense and durable color but also with their structural robustness under technologically demanding conditions. Owing to these features, metal phthalocyanines have found broad application in coating systems, polymer composites, protective layers, optical materials, and other advanced functional products [5]. In cobalt phthalocyanine derivatives, the nature of the central metal atom contributes significantly to electronic configuration, intermolecular packing, and overall structural stability, which in turn affects the pigment's performance in real materials.

A key factor controlling the functional behavior of phthalocyanine pigments is their solid-state organization. Earlier crystallographic and powder X-ray diffraction studies demonstrated that phthalocyanines can exhibit distinct polymorphic forms and different molecular packing motifs, including herringbone-like arrangements and modified stacked architectures [6]. In cobalt phthalocyanine systems, structural variations between crystalline forms are especially important because they influence intermolecular interactions, crystallinity, and phase stability [7]. Therefore, X-ray diffraction remains one of the most informative methods for evaluating the phase composition and crystal structure of both unmodified and chemically modified phthalocyanine pigments.

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At the same time, practical application of conventional phthalocyanine pigments is often limited by relatively low polarity, a tendency toward aggregation, and insufficient compatibility with some binder systems, especially in waterborne and hybrid formulations [8]. For this reason, chemical modification of the phthalocyanine framework with polar or multifunctional substituents has become an effective strategy for improving dispersibility, interfacial behavior, and adhesion in formulated systems. Phosphorus- and nitrogen-containing groups are of particular interest because they can introduce additional polar centers, alter intermolecular interactions, and affect crystal packing without necessarily destroying the main macrocyclic core [9]. In this context, the incorporation of a diamidophosphate fragment may lead to substantial changes in both the chemical environment and the phase structure of cobalt phthalocyanine pigments.

Recent studies on modified phthalocyanine-based pigments and coating-related systems have shown that structural tuning can improve heat resistance, weathering behavior, dispersibility, and compatibility with surrounding matrices [10]. Surface modification and hybridization with inorganic or functional fragments have also been shown to affect morphology, phase composition, and thermal stability, thereby broadening the technological relevance of phthalocyanine pigments in high-performance applications [11]. However, despite the growing interest in functionalized phthalocyanines, the phase-state consequences of diamidophosphate modification in cobalt phthalocyanine pigments remain insufficiently described, especially from the standpoint of powder X-ray analysis and structure-related interpretation.

In addition, earlier regional studies on diamidophosphate-containing cobalt and nickel phthalocyanine pigments have mainly focused on thermal behavior and general physicochemical characteristics rather than on detailed phase interpretation from diffraction data [12]. This indicates that the structural effect of diamidophosphate incorporation still requires a more explicit X-ray-based assessment. Therefore, the present study aims to evaluate the phase composition, crystallinity, and structural changes induced by diamidophosphate modification in a cobalt phthalocyanine pigment on the basis of its X-ray diffractogram. Such analysis is important for understanding how chemical functionalization influences crystal organization and, consequently, the potential performance of the pigment in functional coating and composite systems.

MATERIALS AND METHODS.

The material investigated in this study was a modified cobalt phthalocyanine pigment containing a diamidophosphate fragment as a functional substituent. Structural characterization of the obtained pigment was performed

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using X-ray diffraction (XRD) analysis in order to assess its phase composition and crystalline organization.

The diffraction pattern was evaluated through qualitative analysis of the principal and secondary reflections, with particular attention given to peak distribution, relative peak intensity, and the overall shape of the diffraction background. This approach was used to identify the presence of ordered crystalline domains, partially disordered regions, and possible structural heterogeneity associated with the chemical modification of the cobalt phthalocyanine framework.

The interpretation of the XRD data was carried out primarily on a qualitative basis because the available diffractogram image did not include a complete numerical dataset of individual 2θ values, corresponding interplanar spacings, or indexed reflections required for full quantitative phase analysis. Accordingly, the analysis focused on the general features of the diffraction pattern, including the number of observable reflections, their relative intensity, peak broadening, and the coexistence of sharp and diffuse diffraction features.

Special attention was paid to the preservation of the characteristic reflections associated with the cobalt phthalocyanine core and to the appearance of additional peaks that could indicate structural reorganization induced by diamidophosphate incorporation. Broadened reflections were considered as possible evidence of reduced crystallite size, lattice disorder, or the presence of partially amorphous regions. Despite the absence of a complete tabulated diffraction dataset, the XRD pattern provided sufficient structural information to evaluate the influence of modification on the phase state and crystal organization of the synthesized pigment.

RESULTS AND DISCUSSION.

The phase composition and structural organization of the synthesized diamidophosphate-modified cobalt phthalocyanine pigment were evaluated by X-ray diffraction analysis. As shown in Figure 1, the obtained diffractogram exhibits a structurally complex pattern characterized by multiple diffraction reflections with different intensities and peak shapes. The presence of several pronounced reflections indicates that the synthesized pigment retains a considerable degree of crystallinity. At the same time, the elevated diffraction background and the coexistence of broadened reflections suggest that the material also contains partially disordered or weakly crystalline regions.

The phase composition and structural organization of the synthesized pigment were evaluated by X-ray diffraction analysis, and the obtained diffractogram is discussed below.

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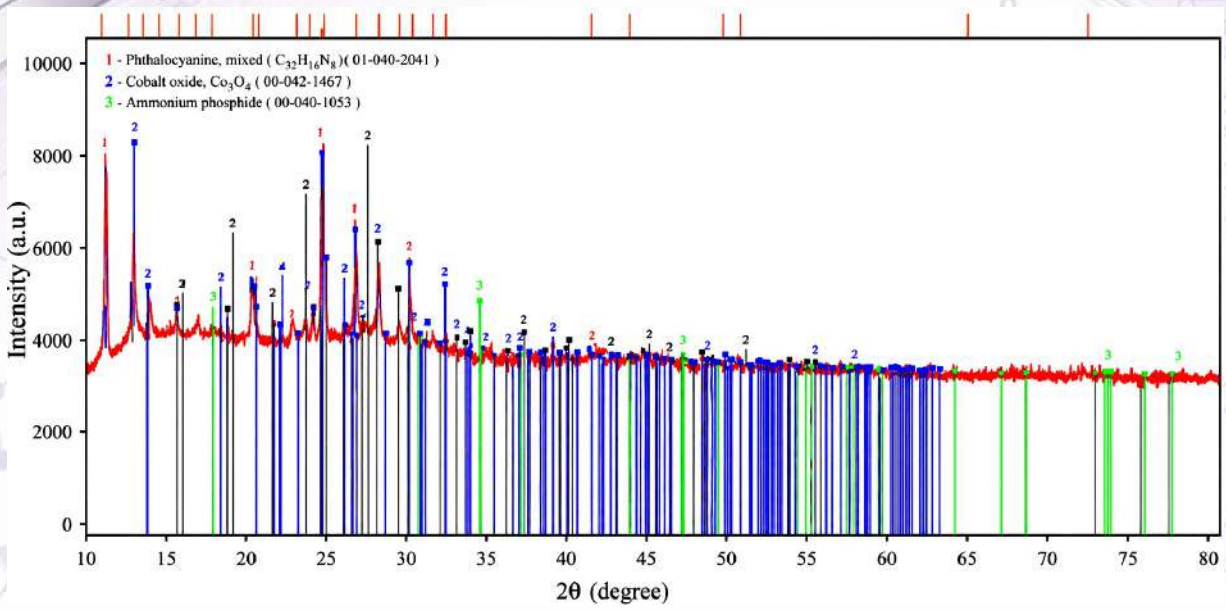


Figure 1. X-ray diffractogram of the diamidophosphate-modified cobalt phthalocyanine pigment

The major diffraction peaks observed in Figure 1 can be attributed to the preserved crystalline fragments of the cobalt phthalocyanine framework. This result indicates that the modification process did not destroy the principal cobalt-centered macrocyclic core. The retention of this structural unit is of particular importance because the chromatic behavior, electronic delocalization, and intrinsic stability of cobalt phthalocyanine pigments are closely associated with the integrity of the macrocyclic conjugated system. Therefore, the diffraction data confirm that the synthesized product preserved the essential structural identity of cobalt phthalocyanine after chemical modification.

In addition to the main reflections, Figure 1 also reveals secondary diffraction features, which may be associated with structural changes induced by the incorporation of diamidophosphate groups. The introduction of phosphorus- and nitrogen-containing functional fragments can modify intermolecular interactions, influence crystal packing, and disturb the regular stacking of phthalocyanine macrocycles. As a consequence, the appearance of additional reflections or variations in the relative intensity of the principal peaks can be interpreted as evidence of lattice rearrangement caused by chemical functionalization. These observations suggest that the modification affected not only the chemical environment of the pigment but also its phase organization in the solid state.

A characteristic feature of the diffractogram is the simultaneous presence of sharp, intense peaks and broader, less resolved reflections. The sharp diffraction maxima are indicative of relatively well-ordered crystalline domains, whereas the broadened peaks are commonly associated with smaller coherent

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domains, reduced crystallite perfection, or partially amorphous regions. This structural heterogeneity is consistent with the expected effect of peripheral diamidophosphate substituents, which can partially disrupt the ideal molecular packing of cobalt phthalocyanine while preserving the main macrocyclic framework. As a result, the modified pigment may be regarded as a hybrid system containing both ordered crystalline regions and less ordered structural domains.

Such a phase arrangement is expected to influence the practical behavior of the pigment. The preserved crystalline core is likely to maintain the characteristic color intensity and structural stability of cobalt phthalocyanine, whereas the modified and less ordered regions may increase surface polarity and improve compatibility with polymeric binders and composite matrices. From an application standpoint, this combination of structural stability and surface modification is advantageous for the development of high-performance pigments for coatings, polymer-based materials, and other advanced functional systems.

Overall, the X-ray diffraction pattern presented in Figure 1 demonstrates that the synthesized material should not be regarded as a simple single-phase compound. Rather, it represents a structurally modified hybrid pigment in which the crystalline cobalt phthalocyanine framework is retained while diamidophosphate incorporation gives rise to additional phase features and partial lattice reorganization. These results confirm the successful course of the modification process and provide structural evidence for the formation of a new functional pigment system.

CONCLUSION.

The present X-ray diffraction analysis demonstrated that the diamidophosphate-containing cobalt phthalocyanine pigment exhibits a structurally complex and heterogeneous phase organization. The persistence of the principal diffraction reflections characteristic of cobalt phthalocyanine confirms that the macrocyclic cobalt-centered framework remained structurally preserved during the modification process. Simultaneously, the appearance of additional diffraction features and the variation in peak profiles provide clear evidence that diamidophosphate incorporation induced partial reorganization of the crystal lattice and altered the solid-state arrangement of the pigment.

These results indicate that the modification affected not only the chemical functionality of the material but also its crystallinity, intermolecular packing, and phase state. Rather than forming a simple single-phase product, the synthesized pigment developed into a hybrid structural system composed of a retained phthalocyanine crystalline core and newly reorganized domains associated with phosphorus-containing functional fragments. This finding is important because it demonstrates that diamidophosphate modification can be used as an effective

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strategy for tuning the structural characteristics of cobalt phthalocyanine pigments without destroying the parent chromophoric framework.

From the standpoint of practical application, such a structural combination is highly significant. The preserved crystalline cobalt phthalocyanine domains are expected to maintain the inherent color strength, molecular rigidity, and stability typical of metal phthalocyanine pigments, whereas the modified regions may enhance surface polarity and improve interaction with polymeric binders, coating matrices, and composite systems. Thus, the observed phase transformation is not merely a structural phenomenon, but a potentially beneficial factor governing the technological performance of the pigment.

In summary, the XRD results confirm the successful formation of a diamidophosphate-modified cobalt phthalocyanine pigment with hybrid phase characteristics and altered crystal organization. The combination of structural integrity and functional modification suggests that this material is a promising candidate for use in advanced coatings, high-stability polymer composites, and other functional applications where durable color properties, phase stability, and improved matrix compatibility are required.

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