MS40 P01

Synthesis, characterisation and X-ray study of Ni(II) complex : $[Ni(H_2P_2O_7)(C_{12}H_8N_2)_2].2.5H_2O$

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Keywords: **Structure compounds, characterization method, magnetic crystal structures.**

Investigation of novel organic phosphate complexes represents the intense interest of chemical research because of their diverse practical applications.

This complex has been characterized by X-ray diffraction, IR spectral analysis and UV-vis spectroscopic. The natural elements in the complex are detected by the EDX on a scanning electron microscope. The thermal analysis (TG, DTA) shows that the dehydratation of compound occurs in agreement with the structural features.

The title complex was prepared by hydrothermal crystallization in a sealed vessel from ethanolic solutions of nickel nitrate, 1,10-phenanthroline hydrate, phosphoric acid and water.

The structure was determined by X-ray diffraction on single crystal. This compound crystallizes in the triclinic space group P-1 with a = 10.285(2) Å,
b = 10.510(3) Å, c = 12.775(3) Å, α = 88.06(2)°, β = 77.87(2)°, γ = 89.26(2)°,
V = 1349.2(5) $Å^3$, Z = 2 and refined to R = 0.042 and wR = 0.012.

Crystal structure of $[Ni(H_2P_2O_7)(C_{12}H_8N_2)_2].2.5H_2O$ is composed of nickel complexes and water molecules. Each complex is connected to two others by means of hydrogen bonding and weak π-π stacking interactions, to form a bi-dimensional framework, which delimits b-axis tunnels, where water molecules are located.

The Ni^{II} ion is coordinated in a distorted octahedral arrangement by one O and three tertiary N atoms in equatorial positions, and by O and N atoms in axial positions.

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MS40 P02

A Refinement Target Directly Using the Experimental Phase Information from SIRAS experiment

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Keywords: automatic model building and refinement; direct use of experimental phase information; multivariate refinement target

Previously, the direct use of prior phase information from a single-wavelength anomalous diffraction (SAD) experiment with a multivariate likelihood function applied to automated model building with iterative refinement was proposed [1] and shown to extend the limits for successful model building [2].

We have derived a multivariate likelihood function that directly incorporates the experimental phase information from a single isomorphous replacement with anomalous scattering (SIRAS) experiment, accounting for the correlations between the observations and the models. The implementation of the derived likelihood function requires multi-dimensional numerical integration, leading to the necessity of approximations in order to achieve an efficient implementation. Based on the properties of the three-dimensional integral of the SIRAS function, we have proposed an algorithm for the evaluation of this integral and we have implemented the algorithm in REFMAC5. The algorithm and the performance of the SIRAS function have been tested on several SIRAS datasets, yielding satisfactory results.

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MS40 P03

Crystal Structure Of 2-[2-(-Amınophenoxy) Ethoxy]-N-[(1e)-2,3,5,6,8,9,11,12-Octahydro-1,4,7,10,13-Benzopentaoxacyclopentadecın-15-Ylmethylene]Anılıne

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The title compound, $C_{29}H_{34}N_2O_7$, is a substituted monotopic benzo-15-crown-5-ether ligand. It belongs to the space group $P2_1/a$ with cell parameters a = 8.9857(6), b = 25.0353(17), c = 12.6979(9)Å and β = 109.730(1)°. The intermolecular N-H…O hydrogen bonds are dominantly effective in stabilizing the crystal structure. The N-H…O intermolecular hydrogen bonds link the molecules, forming infinite one-dimensional chains running approximately parallel to the *a*-axis. The relative macrocyclic inner-hole size is estimated to be 1.44 Å. The substituent and benzocrown ether precursors about the C=N imine bond reveals a *trans* planar (1*E*) configuration.

MS40 P04

AMPLIMODES: a computer program for the symmetry-mode analysis of structural phase transitions.

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Keywords: structural phase transitions, symmetry-mode analysis, Bilbao Crystallographic Server

The main signature of a displacive phase transition is the appearance of a symmetry-breaking distortion (with respect to the high symmetry phase) that is mainly caused by the freezing of the so-called *primary* mode, associated with the order parameter. In general, *secondary* modes are also triggered at the transition and can have non-zero amplitudes in the distorted structure. The symmetry-mode analysis of a structural phase transition results in the calculation of the amplitudes of the symmetry modes frozen in the distortion, *i.e.* to the determination of the