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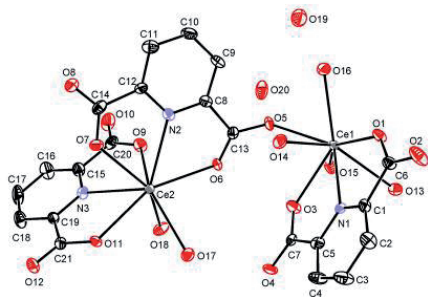
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**Structure of a polymeric Ce(III) complex containing pyridine-2,6-dicarboxylic acid**

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Coordination polymers of rare earth elements have received significant attention in recent years because of their potential optical, magnetic, and porous properties, especially for the carboxylates [1–4]. The large ionic radii of rare earth elements together with the coordination flexibility of lanthanide ions can lead to unusual structural topologies and new framework families [5].

Here we report the synthesis, characterization and crystal structure of the polymeric  $\{[Ce(pydc)_3(H_2O)_8] \cdot 2H_2O\}_n$  complex (**I**), obtained from the reaction of Cerium(III) nitrate with the pyridine-2,6-dicarboxylic acid, dipicolinic acid (pydcH<sub>4</sub>) and 2-aminopyrimidine (ampy) in 1:1:1 molar ratio in basic media. Polymeric complex was characterized by FT-IR spectroscopy and X-ray diffraction. X-ray crystal structural analysis reveals that the compound belongs to the triclinic space group  $P\bar{1}$  with cell parameters  $a = 10.407(4)$  Å,  $b = 11.795(5)$  Å,  $c = 13.770(6)$  Å,  $\alpha = 93.852(2)^\circ$ ,  $\beta = 111.142(2)^\circ$  and  $\gamma = 111.105(2)^\circ$ . The molecular structure consists of two crystallographic independent pairs of Ce<sup>III</sup> ions in the unit cell (Fig. 1). The coordination polyhedron of the ten-coordinated Ce1 ion is a distorted bicapped square antiprism comprised of O1 and O2 bridged atoms from pydc ligand coordinated to the Ce1 ion of the neighboring unit, N1,O3,O4 atoms of the one dipicolinate ligand, bridged O5 atom of pydc ligand coordinated to the Ce2 ion of another neighboring unit, O13, O14, O15 and O16 atoms of the water molecules. The Ce2 ion is in slightly distorted tricapped trigonal prism being coordinated by N2, O6, O7 and O8, O11 and N3 atoms from two dipicolinate ligands, bridged O11 atom from pydc linked to the Ce2 ion of the neighboring unit, O17 and O18 atoms of the water molecules. In the crystal structure, a wide range of noncovalent interactions consisting of hydrogen bonding (of the types of O–H...O and C–H...O) and ion pairing interactions connect the various components into a supramolecular structure.



**Fig. 1.** ORTEP plot showing the coordination environments of cerium ions in **I**.

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**Reciprocal space statistical thermodynamics of inhomogeneous disordered systems**

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Within the last decades a lot of efforts were made in order to understand the nature of dynamical heterogeneities in disordered systems, e.g. supercooled liquids, amorphous alloys. Nevertheless the nature of the amorphous state formation, a fundamental problem of condensed matter physics, is not completely understood.

It has been recently shown [1] that the dynamic origin of heterogeneous dynamics might be a result of critical-like fluctuations of static structural order. This is a concept that counters the currently accepted trend.

Here we present a reciprocal-space approach for inhomogeneous systems, based on the ring approximation [2], [3]. This concept deals with cooperative reciprocal-state modes and takes into account their statistical coupling, both in atomic interaction and in mutual arrangement of particles, much unlike traditional real-space statistical thermodynamic approaches.

Using the ring approximation in the framework of kinetic atomic density functional approach [4], we describe configurational self-organization in the amorphous state. The Fourier transform of the relaxation time is given by the following expression:

$$\tau(\mathbf{q}, T) \sim -kT/[D_0(T)q^2 V_{eff}(\mathbf{q}, T)], \quad (1)$$

where  $\mathbf{q}$  is a reciprocal lattice vector, temperature-dependent coefficient  $D_0(T)$  accounts diffusive properties of the system,  $V_{eff}(\mathbf{q}, T)$  is the “renormalized” effective pairwise interaction potential [1], and it is taken into account that interference of atomic interaction modes with different wave vectors takes place. In the mathematical expression above it is also assumed that the temperature range is significantly lower than the structural instability point, also called spinodal point.

Equation (1) leads to the conclusion that the dominant mode, corresponding to the minimal negative value of  $V_{eff}(\mathbf{q}, T)$ , develops the most intensively. For the Dzugutov-like potential, widely used in simulations of the amorphous state, the function  $V_{eff}(\mathbf{q})$ , exhibits a flat region of the dominant modes for a certain range of potential parameters. Consequently, a set of these modes possesses the same value of relaxation time. This corresponds to formation of a highly inhomogeneous structural state. Interference of the dominant modes leads to the long-living ordered structural states, e.g., clusters, recently revealed by X-ray cross-correlation analysis [5] of coherent scattering data.

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