

## Synthesis, crystal structure and optical properties of new (Nd, Sm) and other lanthanide (Ln=Pr) complexes with 1,10-phenanthroline and thiocyanate.

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New types of neodymium, samarium and other light lanthanide (Pr) mixed complexes with thiocyanate (NCS) and 1,10-phenanthroline (Phen) were synthesized in solution and as crystals. It was found that these complexes crystallized with the formulae: (phen)·[Nd(phen)<sub>2</sub>(NCS)<sub>4</sub>] (**1**) and [Ln(phen)<sub>3</sub>(NCS)<sub>3</sub>]·EtOH (Ln=Sm(**2**), Pr(**3**)). The Pr and Sm complexes are isostructural (space group *P*2<sub>1</sub>/*n*), but the Nd compound was different (space group *P*2<sub>1</sub>/*n*). Compound (**1**) crystallizes in a monoclinic system with space group *P*2<sub>1</sub>/*n* and the following unit cell parameters: *a*=12.097(2), *b*=16.444(3), *c*=19.202(3) Å, β=93.46(2)

The optical spectra of these two types of rare-earth compounds were performed at room and low temperatures in order to understand the electrostatic nature of the Ln<sup>3+</sup>N coordination bonds. The high values of absorption spectral intensities at 293K for Nd<sup>3+</sup> or Pr<sup>3+</sup> show low symmetries for these metal centres. The absorption spectrum analysis at 4.2K and the correlation of the results with the IR spectra of the monocrystals of (phen)·[Nd(phen)<sub>2</sub>(NCS)<sub>4</sub>] and [Pr(phen)<sub>3</sub>(NCS)<sub>3</sub>]·Et(OH) make it possible to account for vibronic transitions. The observed Stark splitting of f–f transitions for Ln<sup>3+</sup> ions in the emission spectra at 77K for Sm<sup>3+</sup> is in agreement with that predicted by group theory for a single low-symmetry Ln<sup>3+</sup> ion site. In the absorption spectra, a 'red shift' was observed for hypersensitive transitions of lanthanide ions. The variation of the spectroscopic parameters of the title compounds, calculated based on the absorption spectra, the nephelauxetic ratio β, Sinha's parameter δ and their correlation with the nature of the Ln<sup>3+</sup>N bond, are discussed.

### Słowa kluczowe

neodymium, atom, Thiocyanate, UV–vis spectroscopy, crystal structure

Adres publiczny

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