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Nd^{3+} and Yb^{3+} complexes with N-(diphenylphosphoryl)pyrazine-2-carboxamide as UV-NIR radiation converters and single-ion magnets.

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The increased interest in designing bifunctional magnetic-luminescent compounds stems from their promising application potential. Appropriately designed lanthanide coordination compounds were found suitable for this purpose. This work describes the structural, optical and magnetic properties of photostable lanthanide coordination compounds (Nd, Yb) with *N*-(diphenylphosphoryl)pyrazine-2-carboxamide (HL) acting as an antenna. Optical properties of the compounds were characterized by IR, high-resolution absorption and emission spectroscopies at 300, 77 and 5 K. The trinuclear coordination compounds (labeled as **Na_2LnL_4**), with a crystal structure stiffened by eight oxygen bridges with eight-coordinated lanthanide ion, as well as six- and seven-coordinated Na ions, were found to be excellent converters of UV radiation into the NIR. The ligand-to-metal energy transfer mechanisms in **Na_2NdL_4** were discussed. **Na_2YbL_4** reached the highest (= 5.8%) overall emission quantum yield among the coordination compounds of Yb^{3+} with organic ligands in solid state. The static and dynamic magnetic properties of **Na_2NdL_4** and **Na_2YbL_4** were studied, revealing that the compounds exhibit behavior of field-induced Single Ion Magnets (SIMs) with the effective energy barrier value of 27.4 K **(Na_2NdL_4)** and 26.2 K (**Na_2YbL_4**). The anisotropic barrier was extracted from static magnetism and optical properties analysis, giving an insight into the magneto-optical correlation. We demonstrated that proper design of ligand structure and coordination compound architecture allows to obtain molecular magnets with optimized infrared emission.

Słowa kluczowe

Lanthanide, Phosphorylated carboxamides, Energy transfer, Single-ion magnet, Luminescence, Crystal structure

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