

The effect of the outer-sphere cations on the photophysical and magnetic properties of rare earth complexes with 2,2,2-trichloro-N-(diphenylphosphoryl)acetamide

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Streszczenie

Two series of rare earth coordination compounds have been synthesized (**Na[RE(L₄)]** (labeled as **1RE**) and **PPh₄[RE(L₄)]** (labeled as **2RE**), where RE = Y³⁺, Eu³⁺, Tb³⁺, L = 2,2,2-trichloro-N-(diphenylphosphoryl)acetamide) to determine the possibility of modifying their photophysical and magnetical properties by changing the counterion. The crystal structure of **1RE** was determined based on the single-crystal X-ray diffraction and the crystal structure of **2RE** was determined based on quantum chemistry computational procedures. Characterization of the physicochemical properties of the compounds was carried out using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), ¹H and ³¹P NMR spectroscopy as well as FT-IR, absorption and luminescence spectroscopy in the temperature range of 300 - 77 K. The rate constants of radiative (A_{rad}) and non-radiative (A_{nrad}) transitions, intrinsic (Q^{L_n}_{L_n}) and overall (Q^{L_n}_{L_n}) emission quantum yields, sensitization efficiency (η_{sens}), the experimental and theoretical intensity parameters (Ω_λ), the forward (W_s, W_t) and backward (W_{b^s}, W_{b^t}) intramolecular energy transfer (IET) rates were determined. Magnetic properties of Tb³⁺ compounds were studied in a constant field of 0.5 T in the temperature range of 1.8–300 K. Dynamic AC magnetic susceptibility measurements were carried out as a function of temperature and frequency for **1Tb** and **2Tb**. Only in the case of **2Tb**, in the presence of an external DC field, a slight temperature dependence of in-phase χ' and out-of-phase χ'' susceptibility was recorded. Based on experimental and theoretical results, the significant effect of counterion on the photophysical and magnetic properties of RE chelates has been demonstrated and clarified, providing valuable guidance for the design of bifunctional electromagnetic radiation converters.

Słowa kluczowe

Lanthanide, Crystal structure, Luminescence, Theoretical calculations, Magnetic properties

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