Hydrated halogenides of Eu(II): structure, spectroscopy and charge density analysis

Autorzy

Przemysław Starynowicz

Rok wydania

2024

Czasopismo

New Journal of Chemistry

Numer woluminu

48

Strony

15921-15934

DOI

10.1039/d4nj02731k

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Five hydrated halogenides of divalent europium, $EuCl_2 \cdot 2H_2O$ (tagged as **Cl2**), $EuCl_2 \cdot 6H_2O$ (**Cl6**), $EuBr_2 \cdot H_2O$ (**Br1**), $EuBr_2 \cdot 6H_2O$ (**Br6**) and $EuI_2 \cdot 6H_2O$ (**I6**), were studied herein. The crystals are all isomorphous with analogous compounds of Sr. In **Cl2**, the metal cation is surrounded by 4 Cl^- anions and 4 water molecules; in **Br1**, it is surrounded by 7 Br^- anions and 2 water molecules; and in **Cl6**, **Br6** and **I6**, it is surrounded by 9 water molecules, with infinite $[Eu(H_2O)_6]^{2\infty+}{}_\infty$ chains being formed. Spectroscopic properties of **Cl2**, **Br1**, **Br6** and **I6** were studied. **Cl2** and **Br1** are bright luminophores, whereas **Br6** and **I6** are weak emitters at room temperature. In the latter two compounds, long-wave emissions at about 550 nm were observed and theoretical calculations indicated that this was due to 6,7s → 4f transitions. Additionally, 4f → 4f transitions were observed in the excitation spectra of **Br6** and **I6** recorded at 77 K. Experimental charge density analysis was performed for **Cl6**, and the results show that Eu–O bonds in the $[Eu(H_2O)_6]^{2\infty+}{}_\infty$ polymeric aqua cation are more ionic than those in $[Gd(H_2O)_9]^{3+}$.

Adres publiczny

http://dx.doi.org/10.1039/d4nj02731k

Strona internetowa wydawcy

https://www.rsc.org/