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Luminescent Nitridoalumooxophosphates by High-Pressure / High-Temperature Synthesis

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Intriguing properties of mixed nitride networks have led to a range of viable applications. Nitrido(litho)aluminates, e.g. $Sr[LiAl_3N_4]:Eu^{2+}$ and $Sr_2[MgAl_5N_7]:Eu^{2+}$, are an important part of developments in the lightening industry due to their chemical and thermal stability and luminescence.[1,2] Likewise, nitridosilicophosphates and nitridophosphates contain rare structural motifs.[3,4,5] Dense frameworks and luminescence properties that may improve the quality of specialized light-emitting diodes (LEDs) are highly sensitive to the valence state, coordination spheres, site symmetry of atoms and the concentration of activator ions. Therefore, understanding relationships between luminescent properties and crystal structures is crucial. In investigating the nitride network of nitridoalumo(oxo)phosphates, we combine these characteristics and properties and aimed at luminescent properties like low thermal quenching and a narrow emission due to the structural relationship to nitrido(litho)aluminates. $Sr_2Al_{10}P_8N_{20}O_{4.034}F_{5.094}:Eu^{2+}$ was obtained from $Sr(N_3)_2$, $SrCO_3$, P_3N_5, AlN, EuF_3 and the mineralizer NH_4F by mineralizer-assisted high-temperature high-pressure (HT/HP) synthesis (1400 °C, 5 GPa) with a Walker-type module.[6] The structure was elucidated by SCXRD (single-crystal X-ray diffraction, R1 = 0.0142, wR2 = 0.0327). BVS (bond valence sum) and CHARDI (charge-distribution) calculations indicate mixed anionic positions. The new nitridoalumofluoridooxophosphate crystallizes in space group I-4m2 [a = 11.17902(8), c = 5.1484(1) Å]. TEM SAED (transmission electron microscopy selected area electron diffraction) patterns confirmed the metric and TEM and SEM (scanning transmission electron) EDX (energy dispersive X-ray) coincide with the element ratio obtained by SCXRD. $Sr_2Al_{10}P_8N_{20}O_{4.034}F_{5.094}:Eu^{2+}$ shows a broadband emission with a maximum at 450 nm and a fwhm (full width at half maximum) of 108 nm (5315.0 cm^{-1}). It contains chains of face-sharing $Sr(N/O/F)_{12}$ cuboctahedra, supertetrahedra-like elements composed of ten edge-sharing $Al(N/O/F)_6$ octahedra where Al is positioned on three different crystallographic sites. A three-dimensional network is built by twofold and threefold vertex-sharing PN_4 tetrahedra.

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