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Photoluminescent Behavior of Yttrium and Scandium silioxide solvates

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Lanthanide doped metal siloxide (MSiOx:Ln) materials exploit a wide range of metals from across the periodic table (M = alkaline earth, early transition, late transition, main group, and lanthanide metals) in order to tune their physical and electronic properties. Since there is such a diverse set of compositions available, it is not surprising that $MSiO_x$ materials have found widespread utility in such diverse applications as scintillator applications for medical imaging, X-ray security, deep-well exploration, monitors, and many other everyday applications. In an effort to develop single-source precursors to $MSiO_x$, the reaction of tris(trimethylsilyl)silanol (H-SST) with the group 3 congener amides ($M(NR_2)_3$ where R = $SiMe_3$) was undertaken and found to generate $[(THF)_2M(SST)_3]$ where M = **Sc**, **Y**. The trigonal planar arrangement was in agreement with the previously reported iso-structure $[(THF)_2Ln(SST)_3]$ (**Ln** = lanthanide cations) series synthesized from similar reaction pathways.[1]

As part of the characterization of these compounds, standard analytical data (elemental analyses, FTIR, and XRF) along with multinuclear NMR were obtained to verify solution behavior and purity. To further characterize these compounds, the photoluminescent behavior of these compounds was evaluated. The samples were illuminated with a 365 nm LED to gather the steady state emission and decay time profiles. Emission due to the SST ligand was found to be broad (450 – 650 nm). The non-exponential decay profile for **Y** samples revealed a long (100s of ms), non-exponential decay behavior. This behavior is repeatable on separate samples made a year apart. In comparison, the **Ln** species present typical emission profiles and exponential decays associated with individual Ln^{3+} ions. The **Sc** derivative showed similar behavior but with significantly shorter decay times. It is believed that this behavior is due to a ligand electron reconfiguration in the excited state involving both the SST ligand and the **Y, Sc** ions. Details of the preparation, characterization, and the photoluminescent behavior of these unusual compounds will be presented.

[1] "Synthesis and Characterization of Solvated Lanthanide Tris(trimethylsilyl)siloxides," Timothy J. Boyle, Fernando Guerrero, Roger E. Cramer, Paris C. Reuel, Daniel M. Boye, and Henry L. Brooks, *Inorganic Chemistry* **2022** *61* (12), 5048-5059.