

# Electron Paramagnetic Resonance and DTA Investigation of Cr<sup>3+</sup> in Tris(guanidinium) Hexafluoroaluminate Single Crystals

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Electron Paramagnetic Resonance (EPR) studies of Cr<sup>3+</sup> in single crystals of tris(guanidinium) hexafluoroaluminate,  $[\text{C}(\text{NH}_2)_3]_3\text{AlF}_6$ , have been carried out in the X-band region. A temperature dependent study of the zero-field splitting parameter  $D$  in the range 77–398 K shows the presence of a phase transition, which is supported by Differential Thermal Analysis. In addition, <sup>19</sup>F superhyperfine structure has been observed in the 9.3% naturally abundant <sup>53</sup>Cr isotope hyperfine structure.  $D$  shows a large decrease with increasing temperature. The phase transition brings about a chemical inequivalence in the two chemically equivalent but magnetically inequivalent room temperature  $(\text{CrF}_6)^{3-}$  species. Comparison is made with the alums  $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ , as well as other guanidinium aluminum salts.

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