Synthese, Struktur- und EPR-Untersuchungen an Bis(tetraphenylphosphonium)-bis(1,2-dithioquadratato)oxovanadat(IV), $(Ph_4P)_2[VO(dtsq)_2]$

Synthesis, Structural and EPR Investigations on Bis(tetraphenylphosphonium)-bis(1,2-dithiosquarato)oxovanadate(IV), $(Ph_4P)_2[VO(dtsq)_2]$

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The molecular structure and EPR studies of bis(tetraphenylphosphonium)bis(1,2-dithiosquarato)oxovanadate(IV) are reported. $(Ph_4P)_2[VO(dtsq)_2]$ crystallizes in the monoclinic space group $P2_1/n$ with the unit cell parameters a = 10,9820(2), b = 15,4620(3), c = 14,5050(3) Å, β = 95,700(8)°, Z = 2. The $\boldsymbol{g}$ and hyperfine coupling tensors $\boldsymbol{A}^V$ obtained from the EPR spectra in liquid and frozen solution are used to characterize the properties of the molecular orbital containing the unpaired electron and are compared to those obtained from EHT-MO calculations.

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