S-, X-, Q- und W-Band-Pulver-EPR-Untersuchungen am mononuklearen Au^{II}-Komplex $[Au^{II}([9]anS_3)_2](BF_4)_2$

S-, X-, Q- und W-Band Powder-EPR Investigations on the Mononuclear Au^{II}-Complex $[Au^{II}([9]aneS_3)_2](BF_4)_2$

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Powder-EPR-studies at T = 295, 130 and 13 K of the thiacrown ether Au^{II} complex $[Au^{II}([9]aneS_3)_2](BF_4)_2$ diamagnetically diluted by the corresponding Zn^{II} complex are reported. Due to the small anisotropy of the **g** and the ^{197}Au hyperfine tensor $\mathbf{A}^{Au}$, a large ^{197}Au quadrupole interaction and the noticeable linewidts, the powder spectra show a very complex pattern. Using S-band (2.4 GHz), X-band (9.5 GHz), Q-band (35 GHz) and W-band (94 GHz) frequencies the spectra could be analysed successfully. The spectra were simulated with a computer program which diagonalizes the spin-Hamiltonian matrix exactly. According to EHT-MO calculations most of the spin-density is located in an AuS_4 unit of the distorted AuS_6 unit.