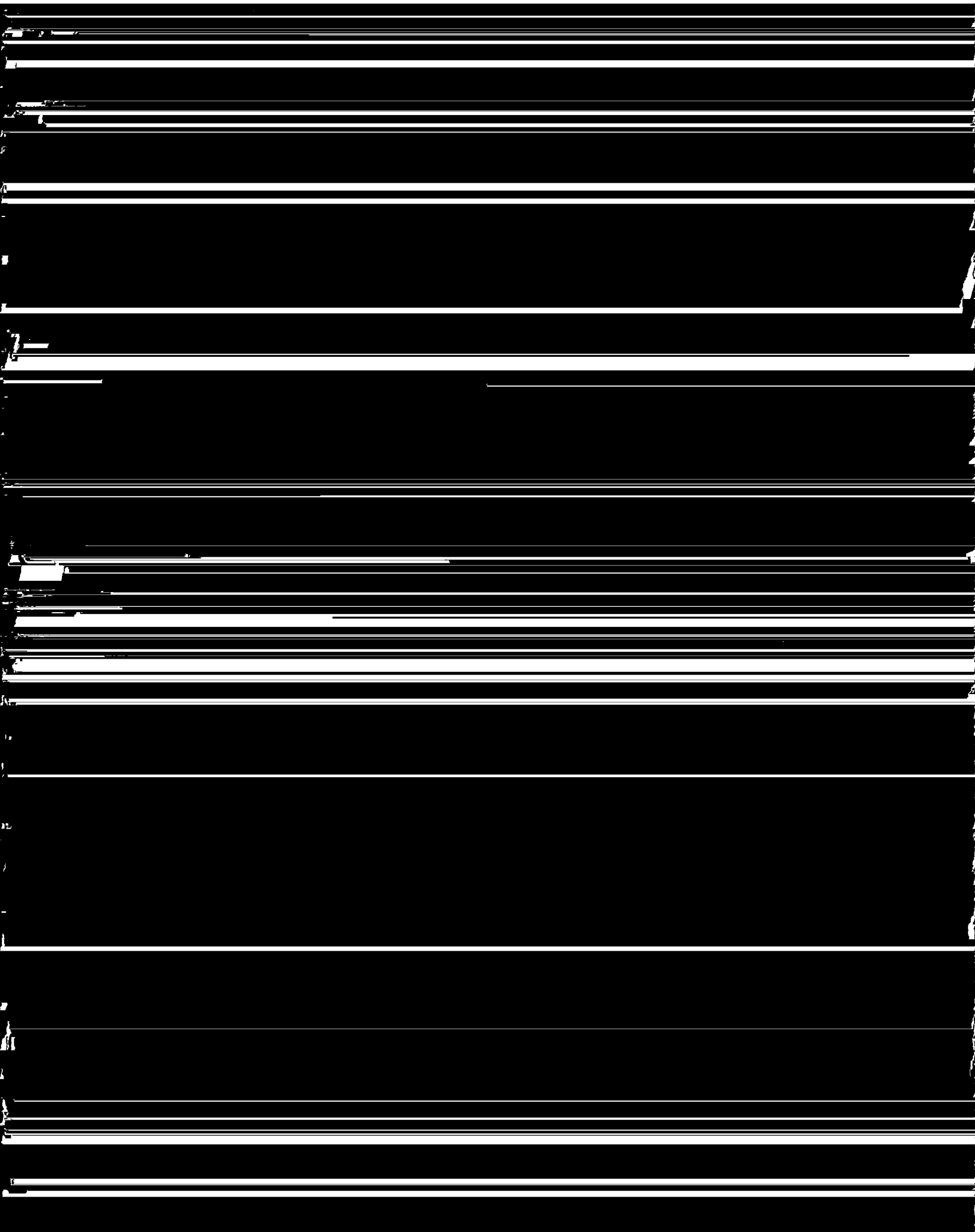
TABLE IV: Experimental and Calculated Values of the g Tensor of Cu(II)-Doped Single Crystals of α-Glycylglycine at 4.2 K

calculated	experimental

The g-tensor principal values were calculated from the equations

$$g_{zz} = 2\sum c_i c_j \langle \psi_i | l_z + 2s_z | \psi_i \rangle \quad (5a)$$