Many relevant properties (including superconductivity and colossal magnetoresistance) of layered materials containing Cu$^{2+}$, Ag$^{2+}$, or Mn$^{3+}$ ions are commonly related to the Jahn–Teller instability. Along this line, the properties of the CuF$_6^{4-}$ complex in the K$_2$ZnF$_4$ layered perovskite have recently been analyzed using a parametrized Jahn–Teller model with an imposed strain [Reinen, D. Inorg. Chem. 2012, 51, 4458]. Here, we present results of ab initio periodic supercell and cluster calculations on K$_2$ZnF$_4$:Cu$^{2+}$, showing unequivocally that the actual origin of the unusual compressed geometry of the CuF$_6^{4-}$ complex along the crystal c axis in that tetragonal lattice is due to the presence of an electric field due to the crystal surrounding the impurity. Our calculations closely reproduce the experimental optical spectrum. The calculated values of the equilibrium equatorial and axial Cu$^{2+}$–F$^-$ distances are, respectively, $R_{\text{eq}} = 193$ pm and $R_{\text{ax}} = 204$ pm, and so the calculated distortion $R_{\text{ax}} - R_{\text{eq}} = 11$ pm is three times smaller than the estimated through the parametrized Jahn–Teller model. As a salient feature, we find that if the CuF$_6^{4-}$ complex would assume a perfect octahedral geometry ($R_{\text{ax}} = R_{\text{eq}} = 203$ pm) the antibonding $\epsilon_2 g^* (-3z^2 - r^2)$ orbital is placed above $b_1 g^* (-x^2 - y^2)$ with a transition energy $E(\epsilon_2 g^* \rightarrow b_1 g^*) = 0.34$ eV. This surprising fact stresses that about half the experimental value $E(\epsilon_2 g^* \rightarrow b_1 g^*) = 0.70$ eV is not due to the small shortening of the axial Cu$^{2+}$–F$^-$ distance, but it comes from the electric field, $E_s(r)$, created by the rest of the lattice ions on the CuF$_6^{4-}$ complex. This internal field, displaying tetragonal symmetry, is thus responsible for the compressed geometry in K$_2$ZnF$_4$:Cu$^{2+}$ and the lack of symmetry breaking behind the ligand relaxation. Moreover, we show that the electronic energy gain in this process comes from bonding orbitals and not from antibonding ones. The present results underline the key role played by ab initio calculations for unveiling all the complexity behind the properties of the model system K$_2$ZnF$_4$:Cu$^{2+}$, opening at the same time a window for improving our knowledge on d$^9$, d$^7$, or d$^4$ ions in other layered compounds.