Single Crystal ESR of Copper Doped $KHCO_3$

Albert Lötz

Department Chemie, Universität München, Butenandtstr. 5 – 13, Haus E, D-81377 München

Reprint requests to Dr. A. L.; Fax: +49 89 2180 77622; E-mail: Albert.Loetz@cup.uni-muenchen.de

Z. Naturforsch. **60a,** 85 – 90 (2005); received September 24, 2004

The principal components of the **g**- and **A**-tensor of $^{63}Cu^{2+}$ obtained from single crystal ESR spectra of copper doped $KHCO_3$ are $g_{zz} = 2.2347(1)$, $g_{yy} = 2.0474(1)$, $g_{xx} = 2.0468(1)$, $A_{zz} = 20.43(2)$ mT, $A_{yy} = 3.22(1)$ mT, $A_{xx} = 2.63(2)$ mT. The unique axes of both tensors are parallel and lie in the mirror plane of the point group of the crystal (2/m). The direction of this axis conforms with the expectation from the structure of the first coordination shell of the K^+ ions. This provides strong evidence for copper entering the K^+ positions without major lattice disturbance. Several of the results presented here are at variance with those of an earlier report on the same subject.

Key words: ESR; Cu^{2+}; Single Crystal; Potassium Bicarbonate.