# Measurement and Calculation of Electric Field Gradients in Hg-Mercaptides *

Torsten Soldner **, Wolfgang Tröger, Tilman Butz, Peter Blaha [a], Karlheinz Schwarz [a] and the ISOLDE-Collaboration [b]

Abteilung Nukleare Festkörperphysik, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig
[a] Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060 Wien
[b] CERN, CH-1211 Genève 23, Switzerland

Z. Naturforsch. **53a**, 404–410 (1998); received October 31, 1997

Electric field gradients (EFG) at Hg were determined in mercury mercaptides $Hg(S(CH_2)_iCH_3)_2$ experimentally for $i \in \{0, 1, 2\}$ using time differential perturbed angular correlation and theoretically for $i \in \{0, 1\}$ with the full potential linearized augmented plane wave code WIEN95. Due to the large unit cells and small hydrogen atoms not full convergence of the plane wave basis set could be reached. Nevertheless, the calculated EFGs agree with experimental values to better than 20%. Furthermore, isolated molecules for $i \in \{0, 1\}$ were investigated theoretically, and strong differences to the values for the crystalline state, especially for the asymmetry parameters $\eta$, were found.

Reprint requests to T. Butz, Fax: +49-341-9 73 27 48.