

An Improved Gas Electron Diffractometer – The Instrument, Data Collection, Reduction and Structure Refinement Procedures

Raphael J. F. Berger, Manfred Hoffmann, Stuart A. Hayes, and Norbert W. Mitzel

Lehrstuhl für Anorganische Chemie und Strukturchemie, Universität Bielefeld, 33615 Bielefeld, Germany

Reprint requests to Prof. Dr. N. W. Mitzel. E-mail: mitzel@uni-bielefeld.de

Z. Naturforsch. **2009**, *64b*, 1259 – 1268; received September 10, 2009

Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

The improvement of a Balzers Eldigraph KD-G2 gas-phase electron diffractometer, previously operated at the University of Tübingen, is reported. The diffractometer was equipped with a state-of-the-art telefocus electron gun, and high-energy radiation-sensitive imaging plates were introduced as detector system. A differential vacuum pumping system separating the diffraction chamber from the electron source was installed. A nozzle for the evaporation of compounds in a temperature range from 25 to 400 °C was constructed and its functionality proven by the structure determination of quinoline. Calibration, data reduction and structure refinement using standard procedures in connection with a selection of literature-known programs are described. The gas-phase structure of quinoline was determined, discussed and compared with *ab initio* and solid-state X-ray diffraction results.

Key words: Gas Electron Diffraction, Gas-phase Structure Determination, Structural Chemistry, Instrumentation, 2-Azabicyclo[4.4]dec-1,3,5,7,9-penta-en