## Charge Density of L-Alanyl-glycyl-L-alanine Based on X-Ray Data Collection Periods from 4 to 130 Hours

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The charge density of the tripeptide L-alanyl-glycyl-L-alanine was determined from three X-ray data sets measured at different experimental setups and under different conditions. Two of the data sets were measured with synchrotron radiation (beamline F1 of Hasylab/DESY, Germany and beamline X10SA of SLS, Paul-Scherer-Institute, Switzerland) at temperatures around 100 K while a third data set was measured under home laboratory conditions (MoK<sub> $\alpha$ </sub> radiation) at a low temperature of 20 K. The multipole refinement strategy to derive the experimental charge density was the same in all cases, so that the obtained charge density properties could directly be compared. While the general analysis of the three data sets suggested a small preference for one of the synchrotron data sets (Hasylab F1), a comparison of topological and atomic properties gave in no case an indication for a preference of any of the three data sets. It follows that even the 4 h data set measured at the SLS performed equally well compared to the data sets of substantially longer exposure time.

Key words: Tripeptides, Charge Density, Topological Analysis, Synchrotron Radiation