MS27-1-5 Charge-density study on α-glycine under high pressure
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Abstract

Nowadays tools for high-pressure experiments become more and more advanced and allow for better quality experiments. Some information, however, is lost during the measurement with the use of diamond anvil cell (DAC), but part of it can be retrieved with a proper data collection and model refinement.

Main objective of this work is to collect high-quality data on α-glycine ($NH3^{+}$–CH2–COO^{-}, $P2_1/n$) at room-temperature under ambient pressure with in-house diffractometer and another under high pressure with the use of synchrotron radiation. Performing refinements of the multipole model against those datasets should give some insights into what are the main challenges of performing charge density studies under high pressure.

In-house diffractometer data was collected with the MoKα radiation with the full completeness up to 1.2 $Å^{-1}$ resolution and high-pressure experiment was carried out under 1.5 GPa and gave completeness of 65% up to the resolution of 1.1 $Å^{-1}$. The collected datasets were reduced, merged and used for refinement of electron density distribution with the application of the multipole model in MoPro[1]. As those abovementioned datasets do not allow for direct comparison, additional file has been artificially created, where the reflections of the high-angle experiment were limited only to those present in the high-pressure experiment. Comparing a model refined on such a dataset with the two based on the original experiments allows for drawing some conclusions on what information is lost when the completeness sharply drops and when the collected raw frames are contaminated with the signal from diamonds and other parts of DAC.

Discrepancies between the obtained models are best illustrated on the differential electron density maps, where two corresponding maps have been subtracted from each other. Employing such a powerful tool, however, should first be preceded with miniscule manual alteration of the final structure files. There are some clearly visible differences between the obtained models refined against the three datasets and they regard the structural, thermal and electronic parameters.

This work was supported by the Foundation for Polish Science, TEAM-TECH Core facility for crystallographic and biophysical research to support the development of medicinal products (co-financed by the European Union under the Regional Development Fund).

References

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