

MS24-2-1 TAAM refinement in dynamical approach against electron diffraction data
#MS24-2-1

B. Gruza¹, P. Brázda², L. Palatinus², P. Dominiak¹

¹Department of Chemistry, University of Warsaw - Warsaw (Poland), ²Institute of Physics of the Czech Academy of Sciences - Prague (Czech Republic)

Abstract

In recent years we observe spectacular development of the methods for 3D electron diffraction (3D ED). People learn how to improve data collection, among others how to diminish radiation damage and how to deal with dynamical scattering. Currently, there are available structures from 3D ED with R-factors below 10% and resolution around $d_{\min}=0.5\text{\AA}$. For such data and refinement with dynamical approach [1] residual density on bonding paths or lone electron pairs regions can be observed. It led us to the necessity to use more sophisticated, aspherical models of electrostatic potential.

We already proposed TAAM refinements against 3D ED data in kinematic approximation [2]. Now TAAM is coupled with dynamical refinement and available in Jana2020 [3]. Here we present refinements of 1-methyluracil crystal structure against $d_{\min}=0.56\text{\AA}$ data with TAAM model in dynamical approach. There is a visible clearing of the residual density map (Figure 1.), also lowering of the maximum and minimum values and further lowering of R-factor. ADPs for non-H atoms become systematically bigger and X-H bonds shorter. In the future we should also be able to go beyond TAAM and refine parameters of the multipole model.

Acknowledgments: This research was funded by National Science Centre, Poland 2020/39/I/ST4/02904

References

- [1] L. Palatinus, V. Petricek, and C. A. Correa, *Acta Crystallogr. Sect. A Found. Adv.*, 2015, vol. 71, pp. 235–244.
- [2] B. Gruza, M. L. Chodkiewicz, J. Krzeszczakowska, and P. M. Dominiak, *Acta Crystallogr. Sect. A Found. Adv.*, 2020, vol. 76, pp. 92–109.
- [3] V. Petricek, M. Dusek, and L. Palatinus, *Zeitschrift für Krist. - Cryst. Mater.*, 2014, vol. 229, pp. 345–352.

Residual density maps

