MS19-2-2 Influence of modelling of disorder on results of Hirshfeld atom refinement of an organo-gold(i) compound
#MS19-2-2

S. Pawlędzio [1], M. Malinska [1], F. Kleemiss [2], S. Grabowsky [3], K. Woźniak [1]

[1]Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw - Warsaw (Poland), [2]Faculty for Chemistry und Pharmacy, University of Regensburg, Universitätsstr. 31, 93053 Regensburg, Germany - Regensburg (Germany), [3]3Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Freiestrasse 3, Bern 3012, Switzerland - Bern (Switzerland)

Abstract
Almost 30% of deposited structures in the Cambridge Structural Database (CSD) are disordered[1]. Usually, it affects only some parts of the molecule, such as freely rotating functional groups, solvents molecules or long side chains. Detecting and modelling of the disorder are important not only in crystallography but also in other related branches of science, including material chemistry, mineralogy, pharmaceutical industry or structural biology. For example, it has been reported that disordered proteins are of important role in binding DNA and signalling cascades[2].
Hirshfeld atom refinement (HAR)[3a],b is a method that uses tailor-made aspherical atomic scattering factors, obtained from the quantum mechanical calculations, to refine atomic positions and their ADPs in the standard least-square refinement. It has been shown that HAR overcomes all the shortcomings of the Independent Atom Model (IAM), yielding more accurate hydrogen atom positions[4] and enabling refinement of hydrogen atom ADPs[5]. Furthermore, HAR was successfully applied to small[6] and big[7], light[6] and heavy[8] molecules. During the last few years, new software for HAR was extensively developed and nowadays modelling of disorder, even for structures with heavy elements, is possible[9a,b].
Our previous study on organo-gold(I) compound and relativistic HAR[10] did not include modelling of disorder. Therefore, here, we will show the reinvestigation of this study with NoSpherA2[9a]. The validation of modelling of disorder with HAR, where wavefunctions were computed using either HF or DFT methods. In some cases also relativistic DKH2 Hamiltonian was used. The impact of modelling of disorder on the results of HAR is analysed in terms of differences of dynamic structure factors, which were calculated from the obtained thermally smeared electron density based on wavefunctions that were computed with or without electron correlation and relativistic effects. The role of modelling disorder is also compared with the effect of treatment of hydrogen atom ADP values, which were obtained from SHADE and as well as from HAR, and atomic anharmonicity of the gold atom.

Acknowledgements: Support from the National Science Centre Poland within PRELUDIUM grant No. UMO-2018/31/N/ST4/02141 is gratefully acknowledged.

References
References:
[1] C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, Acta Crystallographica B, 2016, 72, 171–179.
[2] J. D. Atkins, S. Y. Boateng, T. Sorensen, L. J. McGuffin, Int J Mol Sci., 2015, 16, 19040–19054.
[3] a) D. Jayatilaka, B. Dittrich, Acta Crystallographica Section A, 2008, 64, 383–393. b) S. C. Capelli, H.-B. Bürgi, B. Dittrich, S. Grabowsky, D. Jayatilaka, IUCrJ, 2014, 1, 361–379.
[4] L. A. Malaspina, A. A. Hoser, A. J. Edwards, M. Woińska, M. J. Turner, J. R. Price, K. Sugimoto, E. Nishibori, H.-B. Bürgi, D. Jayatilaka, S. Grabowsky, CrystEngComm, 2020, 22, 4778–4789.
[5] M. Wanat, M. Malinska, A. A. Hoser, K. Woźniak, Molecules, 2021, 26, 3730.
[6] M. Woińska, S. Grabowsky, P. M. Dominiak, K. Woźniak, D. Jayatilaka, Science Advances, 2016, 2, e1600192.
[7] L. A. Malaspina, E. K. Wieduwilt, J. Bergmann, F. Kleemiss, B. Meyer, M. F. Ruiz-López, R. Pal, E. Hupf, J. Beckmann, R. O. Piltz, , A. J. Edwards, S. Grabowsky, A. Genoni, J Phys Chem Lett., 2019, 10, 6973–6982.
[8] L. Bučinský, D. Jayatilaka, S. Grabowsky, The Journal of Physical Chemistry A, 2016, 120, 6650–6669.
[9] a) F. Kleemiss, O. V. Dolomanov, M. Bodensteiner, N. Peyerimhoff, L. Midgley, L. J. Bourhis, A. Genoni, L. A. Malaspina, D. Jayatilaka, J. L. Spencer, F. White, B. Grundkötter-Stock, S. Steinhauer, D. Lentz, H. Puschmann, S. Grabowsky, Chem. Sci., 2021, 12, 1675–1692. b) M. Chodkiewicz, S. Pawledzio, M. Woinska, K. Wozniak, IUCrJ, 2022, 9, 298-315.
[10] S. Pawlędzio, M. Malinska, M. Woińska, J. Wojciechowski, L. Andrade Malaspina, F. Kleemiss, S. Grabowsky, K. Woźniak, IUCrJ, 2021, 8, 608–620.