NoSpherA2 – New possibilities, developments, and challenges

Florian Kleemiss[1], Michael Bodensteiner[1], Horst Puschmann[2], Oleg V. Dolomanov[2]

[1]Universität Regensburg, Fakultät für Chemie und Pharmazie, Regensburg, Germany, florian.kleemiss@ur.de, [2] Olexsys Ltd. Durham University, South Road, Durham, DH1 3LE, UK

The introduction of NoSpherA2 [1] allowed the first-time use of non-spherical scattering factors in routine open-source refinement software, in this case Olex2. Following the initial implementation of Hirshfeld Atom Refinement (HAR)[2] using routine QM software other techniques and software broaden the applicability and feasibility of non-spherical refinements.

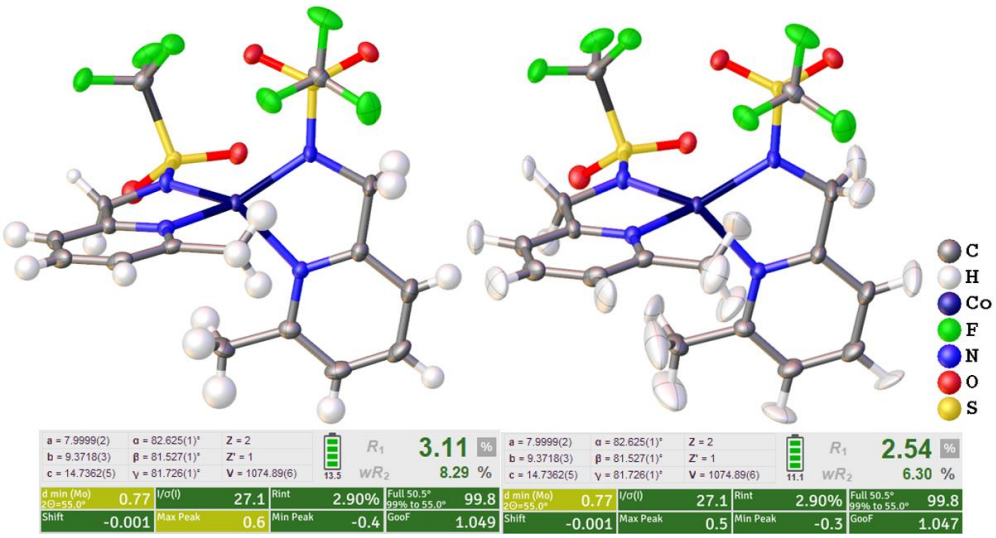

Fig. 1 IAM (left) and HAR (right) with model visualization (top) and refinement statistics (bottom) in Olex2.

The new features include approximations and optimizations for HAR using embedding schemes, linear scaling partitioning or tabulated molecular orbital localization schemes for large molecules, [3] a new Hybrid mode to merge calculations of different levels of theory or methods and a new Independent Atom Model (IAM) using analytical Fourier transformation of the atomic Slater orbital wavefunction from Thakkar et al.[4] Additionally, interfaces to Multipole based databanks (TAAM)[5] are being introduced.

Working with NoSpherA2 on a broader variety of structures showed that there are still open questions arising in the refinement of diffraction data, especially regarding the correction of anomalous dispersion and the treatment of heavy elements. Therefore, new methods are probed to establish a modern calculation of resonance during diffraction and its chemical interpretation based on c

[1] F. Kleemiss, O. V. Dolomanoc, 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. Steinhauser, D. lentz, H. Puschmann, S. Grabowsky, *Chem. Sci.*, 12, 1675-1692 (2021).

[2] a) S. C. Capelli, H.-B. Bürgi, B. Dittrich, S. Grabowsky, D. Jayatilaka, *IUCrJ*, 1(5), 361–379 (2014). b) M. Woinska, S. Grabowsky, P. M. Dominiak, K. Wozniak, D. Jayatilaka, *Sci. Adv.*, 2(5) (2016).

[3] a) F. Neese, F. Wennmohs, U. Becker, C. Riplinger, *J. Chem. Phys,* 152, 224108 (2020). b) J. Bergmann, M. Davidson, E. Okasnen, U. Ryde, D. Jayatilaka, *IUCrJ*, 7(2), 158-165 (2020). c) M. Sironi, A. Genoni, M. Civera, S. Pieraccini, M. Ghitti, *Theor. Chem. Acc.*, 117, 658-698 (2007).

[4] a) T. Koga, K. Kanayama, S. Watanabe, A.J. Thakkar, *Int. J. Quant. Chem.*, 71, 491-497 (1999). b) T. Koga, K. Kanayama, T. Watanabe, T. Imai and A.J. Thakkar, *Theor. Chem. Acc.,* 104, 411-413 (2000).

[5] M. L. Chodkiewicz, S. Migacz, W. Rudnicki, A. Makal, J. A. Kalinowski, N. W. Moriarty, R. W. Grosse-Kunstleve, P. V. Afonine, P. D. Adams, P. M. Dominiak, *J. Appl. Cryst.*, 51, 193-199 (2018).

F.K. acknowledges support by the DFG under grant number KL3500/1-1.