MS19-2-4 NoSpherA2 - From Inorganic to Protein Crystallography
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Abstract
NoSpherA2 [1] – the interface for non-spherical atoms in *Olex2* [2] – was initially capable of performing Hirshfeld Atom Refinement (HAR) [3] for ordered and disordered, mostly molecular, crystal structures. The recent extension of the interface to include databases of multipoles [4] or combine approaches in a "hybrid" mode allow unprecedented speeds of refinements, where known parts of the structure can be described by tabulated or low-level methods, while the remainder can be described using tailor made scattering factors.
The treatment of heavy elements and very large structures like proteins remained time consuming. Two recently implemented methods aim to make these structures refinable using *NoSpherA2* with affordable computational equipment. fragHAR [5] can calculate wavefunctions for large molecules with linear scaling time requirements (see Fig. 1) and help tackle time consuming disorder treatments by describing disordered regions as individual fragments without the need to recompute a wavefunction of the whole structure. While conventional HAR needs exponentially increasing amounts of time with rising numbers of atoms for the wavefunction calculations the fragHAR approach can be fitted using a linear dependence on the atom number. (Fig. 1) Additionally, the use of Effective Core Potentials (ECPs) was introduced into *NoSpherA2*-HAR based on the tight-core treatment of density modelled by ECPs as used in other charge density analysis.[6] This approach allows treatment of large structures and especially heavy elements with relatively little computational resources, since for example Pt can be modelled using 60 electrons in the effective core and therefore reducing the number of orbitals to be calculated and evaluated by 30 in the case of restricted SCF procedures.

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Timing of calculations versus size of structure.