



Your Questions Answered

from SC-XRD Webinar: *IDEAL – Have the Cake and Eat It Too!*

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Q: Is there a model for beryllium available in the database?

A: No

Q: Does standalone shelxle (outside APEX3) offer all the same features?

A: No. All Shelxle versions provide the means to visualize BEDE and LONE instructions. All other features (Invariom partitioning, database access, instruction generation) are only available in APEX3.

Q: What's the increase in parameters used per atom (9 for anis atom becomes ???)

A: No additional parameters are added per atom. Three additional parameters are added globally for scaling purposes. So technically the number of additional parameters per atom is $3/(\text{number of atoms})$.

Q: If you have well-resolved and less well-defined regions in a structure, can/should it be used for part of a structure?

A: Absolutely. We believe this is one of the main benefits of using IDEAL.

Q: What version of APEX3 supports these features?

A: The next version will make IDEAL available.

Q: If I refine bond densities in this way, do I get a better description of unmodeled bonds/contacts that have not been modelled?

A: This strongly depends on the available resolution and data quality.

Q: Does this reorder/replace free variables, i.e. if you already have 10 or so free variables managing a lot of disorder components, will these new ones change them, or append to the end?

A: IDEAL will use the first three free variables it finds. Already defined free variables are not used.

Q: For the CIF files generated, when reviewing, will there be an opportunity to extract the information and confirm reliability/validity of the refinement?

A: We currently don't provide tools to automatically check validity. However, all information required to do validity checks is present.

Q: Can it be used with SQUEEZE?

A: Yes.

Q: Will this help in correct positioning of the H atoms?

A: Possibly. We are looking into the effect of IDEAL on the positioning of hydrogen atoms.

Q: Nice idea. But how to handle imperfection of the crystal?

A: IDEAL has few requirements in terms of resolution and data quality. Poor data will result in little improvement of the model, but there are no minimum requirements.

Q: In the future do you plan to back up the MEASURED electron density into the database? Interesting could be, for example, in case of the frustrated Lewis pairs?

A: We don't have plans to do this.

Q: Does it improve the residual density around heavy atoms, say, lanthanides?

A: Possibly in certain cases, but unlikely in general. IDEAL models bond density and the amount of bond density relative to the overall amount of density around a very heavy atoms is negligible.

Q: Interesting, wondering how it works on molecules exhibiting nitrogen inversion?

A: Nitrogen inversions are certainly challenging. I don't think it is possible to answer the question for all cases of nitrogen inversion. Fast, ammonia like inversion is unlikely to be modelled correctly. However, if you have two distinct conformation, the system can be treated like regular disorder and will work well with IDEAL.

Q: I must apologize for the general question about single-crystal to single-crystal transformations: do we need to fix the orientation matrix to compare two variable temperature structures?

A: That depends on the specific parameters you want to compare.

Q: Can you create and add your own parameters to the database?

A: Technically yes. In practice probably not.

Q: I have a question regarding the multiplicity which we get before execute run. What is a good value range for multiplicity? And tell something about score which we get while indexing?

A: That depends on what you are trying to achieve. If you are only interested in determining whether your synthesis was successful, multiplicity of about 3 at 0.8 Angstroms resolution is probably enough. If you are looking for more detail, you need more multiplicity at higher resolutions. If you want to analyze the charge density of your model you will need very high multiplicity at very high resolutions collected with very well ordered crystals. Probably multiplicities of about 20 at about 0.4 Angstroms resolution. Of course, this also strongly depends on the quality of your crystal. The better your crystal is, the less redundancy is required to get to the same result.

Q: If you use these additional parameters in your model you may improve your R1 simply because of additional parameters refined. Can you still use the Hamilton test to assess the statistical significance of your R1 decrease?

A: Only three parameters are added to the model overall. Those are scaling factors that are applied to all IDEAL parameters equally. The issue of potential overfitting was investigated thoroughly via cross validation. The results were very promising and showed the amount of overfitting gets reduced when introducing the IDEAL model. While not tested explicitly, we do expect equivalent results for Hamilton tests.

Q: Can we use IDEAL to describe polar bonds? 1) How well does it work with polar conjugated systems? 2) When can I look at how the bonds are described now and get information about my bond properties?

A: Polar bonds, even when part of conjugated systems can be modelled. The placement of BEDE pseudo atom along the bond is a good indicator of the polarity of a bond. Bond properties like critical points or ellipticity are not available when using IDEAL.

Q: It seems like we are limited to fragments that are present in the database? is this correct? Also, are we limited to only lighter atoms? What is the largest atom possible to model using IDEAL?

A: The heaviest element present in the database is iodine. However, only few fragments for iodine are present. Mostly those with terminal iodine atoms. The heaviest atom available in a large number of bonding environments is Sulphur. Lone pair density needs to be modelled manually for elements heavier than oxygen due to the poor predictability of lone pair geometry.

Q: Is IDEAL appropriate for structures with disorder? If so what further information can be obtained?

A: IDEAL works well with disordered structures. IDEAL allows us to model each bond individually. Poorly ordered parts of the structures can be left out safely or added manually to improve the phases. Improved phases can then help to model poorly ordered parts.

Q: Do you think the plots generated by IDEAL could be useful to assess the 'strength' of hydrogen bonds?

A: Possibly. We are looking into the effect of IDEAL on the positioning of hydrogen atoms. Looking at hydrogen atoms specifically would be a logical next step.

Q: What would happen with a completely inorganic structure?

A: Most certainly nothing. The partitioning algorithm would determine that no suitable fragments exist.

Q: If you have chiral centers, what happens to the Flack and Parsons values and esd? Do you see them get lower just like the R1 and wR2?

A: Probably not much. The use of Parson Quotients minimizes the influence of systematic model errors on the Flack parameter. The influence of modelling bond density was tested with the invariom model a few years ago and showed no significant reduction of the Flack parameter's esd. While we did not test the impact of IDEAL on the Flack parameter, it is reasonable to assume that the effect would be similarly negligible.

Q: Was IDEAL tested for triple bond $\text{-C}\equiv\text{N}$, how large is correlation with displacement parameters in this case?

A: We have not tested this case specifically yet.