

About the VLD phasing approach and the variance of electron density maps

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The ceremony talk will skip any historical result, and will only deal with two new approaches, obtained in the last two years, which may be of some interest for the crystallographic community.

The first one deals with a new phasing method [1, 2, 3], called *VLD (Vive la Difference)*, based on the properties of new types of difference and hybrid Fourier syntheses [4,5]. Triplet and quartet invariants are no more necessary for phasing: the only necessary tools are the FFT routines. It is possible to obtain, via these new syntheses, good information on the correct difference structure or on the correct hybrid structure even when the model is completely uncorrelated with the target structure. Ab initio crystal structure solution, and/or crystal structure refinement in combination with other methods, are allowed. The available results will be shortly described.

The variance of the electron density maps (observed, difference, and hybrid) is not extensively used in crystallography, even if examples in literature can be found. The problem may be formulated as follows: calculate the variance in any point of a map, for any space group and for any value of CORR, where CORR is the correlation between model and target structure. The problem has been recently solved [6,7]: thus the variance may be calculated at any step of the phasing process for each point of the map. It may be also shown that this concept is useful also in the final steps of the structure refinement.

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