Ind_X: the method

- *Ind_X* program
  - Choice of test volumes
    - Determination of vectors supporting a test volume
      - Generation of triplets of vectors supporting the test volume
        - Determination of tentative bases from a triplet
        - Saving a tentative basis if its quality is high

The main steps of the indexing procedure implemented in *Ind_X*. Indents mark the beginnings of loops.

The procedure implemented in *Ind_X* relies on the volume of primitive cell of the reciprocal lattice. In the ideal case, this elementary volume is a submultiple of volumes of parallelepipeds spanned by reciprocal lattice vectors, i.e., the latter volumes are distributed periodically. The crucial point is to find the period of the distribution obtained from experimental reciprocal lattice vectors, i.e., to get the actual volume of the primitive cell. The primary tool for identification of periodicities in data series is a periodogram. In the considered case, the periodogram can be seen as the frequency of occurrence of particular periods among volumes of parallelepipeds spanned by triplets of the experimental reciprocal lattice vectors. For many experimental data sets, periodograms tend to be noisy and, depending on the data, they may have very different constitutions. Therefore, *Ind_X* extracts a number of test periods. Alternatively, the test volumes can also be indicated by a user; they can be regularly distributed for a systematic search, or particular values can be pointed out based on an inspection of the periodogram or other premises. For each test volume, there is a subset of reciprocal lattice vectors supporting this test volume in the sense that volumes of parallelepipeds spanned by these vectors are close to integer multiples of the test volume. The program estimates the quality of support by an individual vector by checking triplets in which the vector is comprised, and the best vectors constitute the needed subset. The subsequent confinement to this subset eliminates potential spurious reflections and speeds up the program. The supporting vectors are used to construct tentative solutions. The tentative bases of the reciprocal lattice are bases of low-index superlattices of lattices based on triplets of the supporting vectors. The construction of the solutions also includes two standard steps: fitting integer combinations of basis vectors to the supporting vectors and Buerger reduction of the basis. Having a tentative basis, indexing of all experimental reflections is attempted. The result of the attempt is used to quantify the quality of the basis. The basis is saved if it is sufficiently good, i.e., better than other bases. These steps are repeated for all tentative bases constructed from a given triplet of supporting vectors, for all triplets of vectors supporting a given test volume, and for all test volumes.