The Selling Reduction in Crystallography

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Note: Boris Delaunay in his later publications used the Russian version of his surname: Delone. We will follow that choice.

Abstract:
The unit cell reduction described by Selling and used by Delone is explained in a simple form.

Introduction:

The origin of crystallography was the study of minerals (Hauy, 1784). That led to the study of lattices, since it was clear that repetition underlay the structure of crystals. In order to systematize the enumeration of lattices (unit cells), the mathematical procedures of reduction were developed to produce compact descriptions.

(Niggli, 1928), and (Delone, 1933), used reduction methods developed in the 19th century by (Eisenstein, 1851), and (Selling, 1874), respectively. We provide a complete description of the reduction of Selling that can be applied in crystallography.

The Selling Scalars:
As applied to crystallography, the scalars to be reduced by Selling's method are the dot products of the unit cell axes and the negative of their sum (a body diagonal). Labeling these $\underline{a}$,$\underline{b}$,$\underline{c}$, and $\underline{d}$, the scalars are $\underline{b}.\underline{c}$, $\underline{a}.\underline{c}$, $\underline{a}.\underline{b}$, $\underline{a}.\underline{d}$, $\underline{b}.\underline{d}$, $\underline{c}.\underline{d}$. For the purpose of organizing these six in this paper, we describe them as a vector, S, with components, s1, s2, .., s6.

For the purpose of Selling reduction, zero is considered to be negative.

The Tetrahedron:
An alternate description due to (Bravais, 1850), is to consider the scalars as the edges of a tetrahedron formed by the ends of $\underline{a}$, $\underline{b}$, $\underline{c}$, and $\underline{d}$. Thus, $\underline{a}.\underline{b}$ is the label of the edge between the ends of vectors $\underline{a}$ and $\underline{b}$, etc. In the quote below, opposite can refer to a pair of edges of the tetrahedon across the tetrahedron from each other.

The Reduction:
(Delone, Galiulin and Shtogrin, 1975), say "*Select any positive parameter of the tetrahedron and subtract it from the parameter standing on the opposite*

edge of the symbol (the tetrahedron is at all times thought of as spatial), add it to the parameters standing on the remaining four edges, interchange the places of the obtained parameters on two of these four edges, converging to one of the ends of the original edge (it makes no difference to which), and, finally, change the sign of the positive parameter itself being considered."

The goal of Selling reduction is produce a set where all elements of S are negative or zero. By “opposite” here, is meant pairs of scalars that do not have a common element (and are opposite on the Bravais tetrahedron):

b.c and a.d (s1 and s4)
a.c and b.d (s2 and s5)
a.b and c.d (s3 and s6)

Assuming that s1 is positive, the reduction step produces:

(-s1, s2+s1, s5+s1, s4-s1, s3+s1, s6+s1) or
(-s1, s2+s1, s3+s1, s6-s1, s5+s1, s4+s1)

This is continued until all six scalars are negative. This is known to be a “unique” solution.

By “unique” in the previous paragraph, what is meant is that the list of the six scalars is unique. Their arrangement is not unique. There are 24 reflections (permutations that preserve right-handedness) that are all “reduced”. In terms of the tetrahedron, they are the 24 allowed relabeling of the vertices.

Difficulties in Applying the Selling Reduction to the Methods of (Delone, 1933):

The methods of (Delone, 1933), in particular for the identification of Bravais lattice types, have fallen out of favor. (Patterson and Love, 1957), complain that there is no complete description in the literature. It seems to us that our above description of the reduction is simple and complete. So where is the confusion?

First, the identification of lattice types is usually described in terms of matching a reduced set of scalars to a one of the pictures of the 24 different Bravais tetrahedrons (Delone, 1933), corresponding to the various lattice types (such as body-centered cubic, etc.). This is a complex step: the user must “rotate” his figure to agree with each of the types (equivalent to choosing one of the 24 reflections of his figure to match the orientation those of the 24 types that seem possible).

Second, the user must make decisions about how close to zero each of his scalars is. Each zero or near zero generates additional decisions that must be made. Further, the user may need to make a choice as to whether a near zero (negative after reduction) is so close to zero that another reduction should be done with the value considered positive.

The solution of these problems is best dealt with algebraically by considering a lattice to be represented by a point in a vector space, a topic for a forthcoming paper.

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