Faster, Simpler Bravais Lattice Determination in S6

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Building on the work of Selling from 1874, Niggli in 1928 and Delaunay (Delone) in 1933 developed systems for identifying Bravais lattice types. In recent years, most work on Bravais lattices and related topics have concentrated on Niggli's method. Lately, we have reexamined Delone's method, describing it in a six-dimensional space, S6 (for Selling's six parameters, [**b.c, a.c, a.b, a.d, b.d, c.d**]).

We have found that the new method has led to simpler mathematics, simpler computer codes, and faster execution times. Unit cell reduction is faster, calculating distances between lattices is faster, and a new method of determining likely Bravais lattice type is deterministic. We present applications of searching a large database based on unit cell parameters, of Bravais Lattice type determination, and of clustering for serial crystallography.