DC^7, A very efficient lattice comparison metric

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We present a new, highly efficient metric for comparison of crystallographic lattices based on the Dirichlet cell (or Wigner-Seitz cell) which provides a very similar topology to that obtained with the G^6 and S^6 metrics, but without the combinatorial explosions sometimes seen with those metrics. As with G^6, DC^7 begins with Niggli reduction, but instead of comparing the G^6 parameters, [a.a, b.b, c.c, 2 b.c, 2 a.c, 2b.c] or the S6 parameters [b.c, a.c, a.b, a.d, b.d, c.d], the squares of the 13 lengths of the Niggli cell edges, face diagonals and body diagonals considered in finding the Dirichlet cell, [||a||, ||b||, ||c||, ||b+c||, ||b-c||, ||a+c||, ||a-c||, ||a+b||, ||a-b||, ||a+b+c||, ||a+b-c||, ||a-b+c||, ||-a+b+c||] are sorted and the seven shortest taken as an identifying spectrum, corresponding to the distances between the pairs of faces forming the general Dirichlet cell. It is conjectured that the seven shortest of the thirteen lengths are sufficient to characterize the Niggli reduced cell from which they came, but at present it is best simply to retain the original cell along with the derived spectrum rather than try to recover the cell from the spectrum.

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