A false minimum in the refinement of a 9x superstructure. A problem with commensurately modulated structures with a cell volume (2*N*+1) that of a parent structure.

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The possibility of false minima exists when refining commensurately modulated structures. A subset of reflections {g} are stronger than the remainder {g ± *m*q}, *m* = 1 to *M*, where q is a modulation wave vector. For a commensurate structure *N*q is contained in {g} for some *N* and there can be a choice of q. q is chosen so that the average intensity for particular values of *m* decreases as *m* increases.

Bis[μ-bromo-κ-(3,4,5,6-tetrafluoro-2-diphenylphosphinophenyl)palladium(II)] crystallises with dichlormethane as a 9x superstructure, $C_{36}H_{20}Br_2F_8P_2Pd_2.CH_2Cl_2$, *a* 19.5851(3), *b* 20.3668(4), *c* 23.0951(4) Å, α 104.989(1), β 102.553(1), γ 102.556(1) °, *P*-1, *Z* = 9, *T* = 100 K. Reflections were monitored according to |*m*| where $2h - 3k + l = 9n + m$. The parent structure is the Fourier transform of the *m* = 0 reflections and has axes $a_P = {}^1/_9(2a - 3b + c)$, $b_P = {}^1/_9(4a + 3b + 2c)$, $c_P = {}^1/_3(-a + c)$. We can choose q = c* and translations of a_P, b_P, c_P advance the phase of the primary modulation wave by $2\pi m/9$ with *m* = 1, 2, 3 respectively. Each of the 8 non equivalent inversion centres of the parent structure corresponds to a non equivalent inversion centre of the superstructure. For the *N* even case only half the implied non equivalent operations of a parent structure correspond to symmetry operations in the superstructure and false minima imply picking the wrong half.

The false minimum problem can be interpreted as the coherent combination of overlapping reflections of an otherwise incommensurately modulated structure. The choice of global phase ϕ implies a global phase of *m*ϕ for the satellite reflections g + *m*q. A change of ϕ by π leaves true symmetry elements of a commensurate structure unchanged and only alters the structure if *N* is odd. (When *N* is even the origin shifts). Our structure was solved using *SHELX* but features of the initial refinement were unsatisfactory. Changing the phase by π for reflections with odd *m* then recalculating the Fourier gave the correct solution. Improvement in refinement statistics increased with increasing |*m*|.