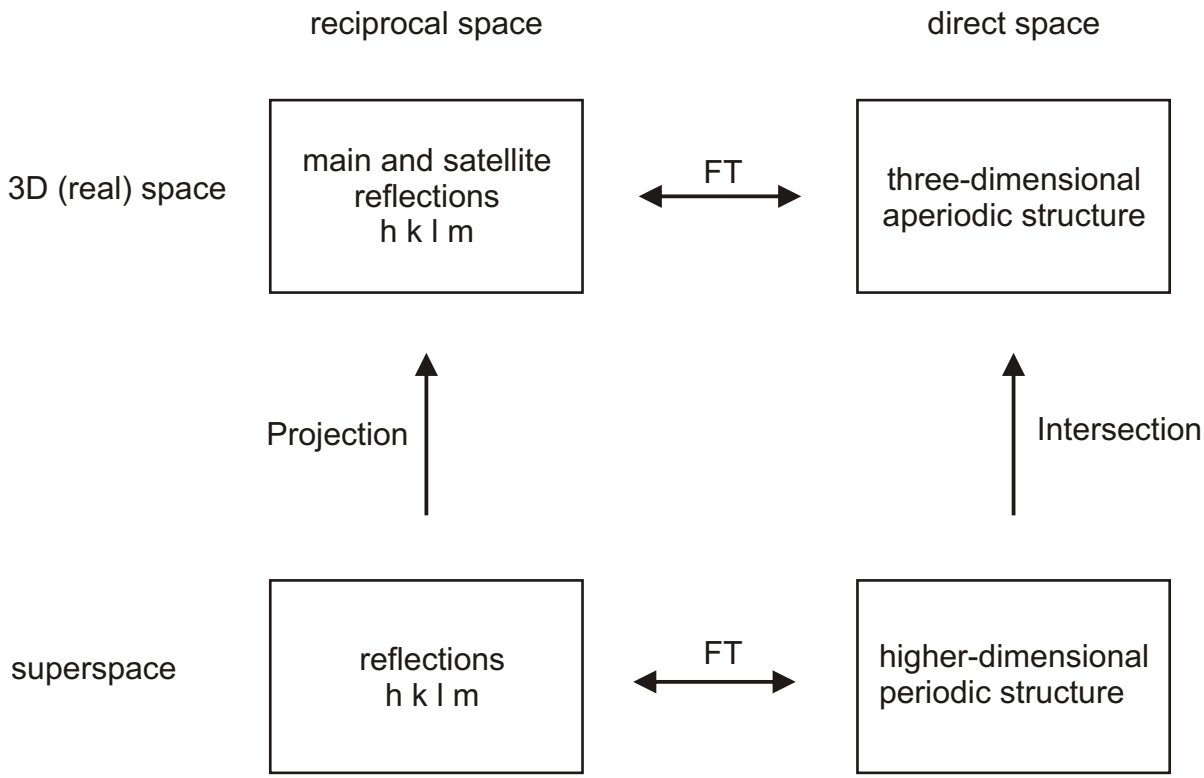

Figure S1

Relation between three-dimensional space and superspace.

The diffraction pattern of an incommensurately modulated structure, observed in three-dimensional reciprocal space (top left), cannot be indexed with three integer values. The positions of the peaks do not coincide with the lattice points of a three-dimensional lattice, i.e., the three-dimensional periodicity is lost (Fig. 3).

Consequently, classical approaches and programs, which are all based on periodicity, will not work.

To overcome this problem, the three-dimensional diffraction pattern is interpreted as the projection (Fig. 6) of a diffraction pattern in higher dimensions (bottom left). In this higher-dimensional space periodicity is restored, the crystal structure can be solved (bottom right).

The aperiodic spatial arrangement of atoms in three-dimensional space can be derived from the superspace crystal structure by an intersection (Fig. 7).

Re-drawn after Fig. 2.4 in van Smaalen (2007).

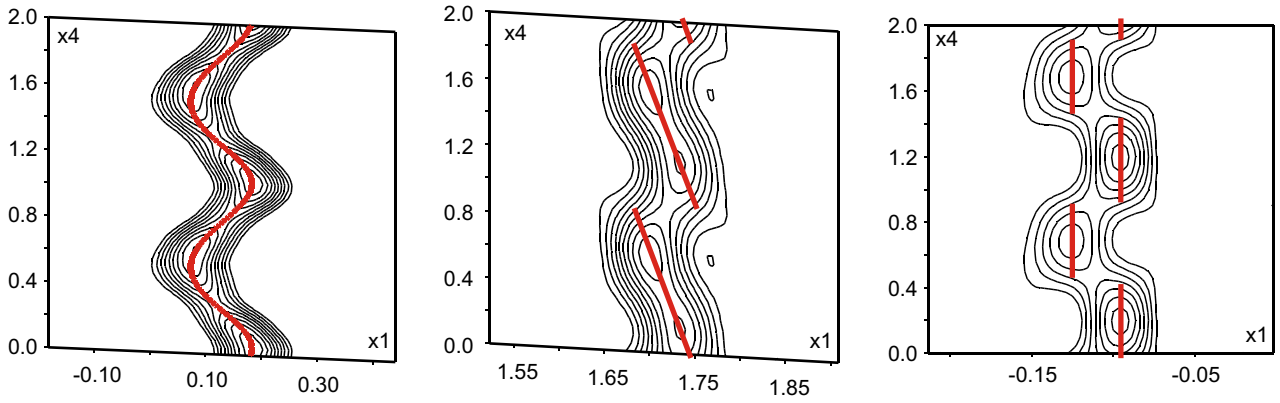

Figure S2

Hypothetical examples of electron densities showing that different types of AMFs can be required to ensure a good fit. On the left, a harmonic modulation function is shown, in the middle a sawtooth function, and on the right a crenel (step-like) function. The decision which type of AMF to apply can be ambiguous and has to be tested in the refinement process.

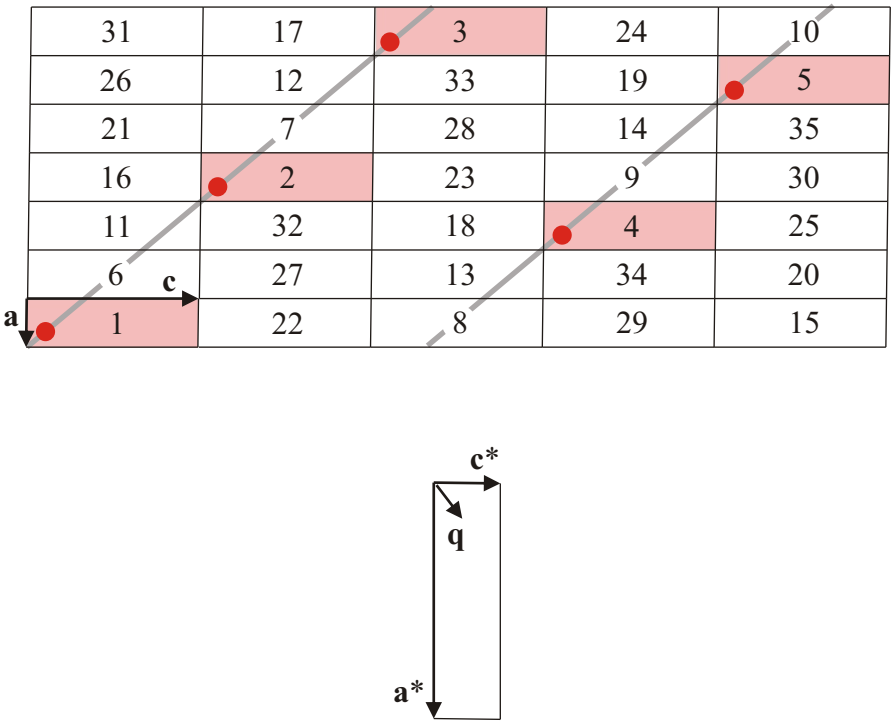

Figure S3

For selecting the molecules along the direction of the modulation one has to proceed "perpendicular" to the direction of the **q**-vector (since the supercell is approximated the direction cannot be exactly perpendicular to **q**). In the case of $C_{19}H_{27}NO_3Si$ not neighbouring molecules are aligned, but molecules which are "one to the right and three up".