Supplementary Materials

Appendix A

Mathematical consequences of placing the origin at the center of mass of the structure

The one-dimensional crystal structure determination problem is substantially simplified by defining the origin at the center of mass of the structure (Shkel *et al.*, 2011), as summarized in this section. In this case, the coordinates of all atoms are related:

$$\sum_{j=1}^{N} x_j = 0 \quad \text{or} \quad \prod_{j=1}^{N} \xi_j = 1 \tag{A1}$$

This relationship preserves the symmetry of equations (1) and (2) in the main text with respect to any permutation of the atomic coordinates. Owing to this symmetry, we can drastically reduce the degree of equations (2) in the main text and (A1) by substituting coordinates ξ_j with the following elementary symmetric polynomials e_h, each of which is defined as a sum of products of all possible combinations of h distinct ξ_j :

$$e_1 = \sum_{j=1}^{N} \xi_j$$

$$e_2 = \sum_{\substack{j,k=1 \\ j \neq k}}^{N} \xi_j \xi_k \tag{A2}$$

…

$$e_N = \prod_{j=1}^{N} \xi_j$$

Note that $e_N = 1$ according to the choice of origin. Owing to this equality, we obtain

$$e_{-h} = \overline{e}_h = e_{N-h}\,, \tag{A3}$$

where the "-h" subscript denotes that ξ_j^{-1} are used in equations (A2) and the bar represents a complex conjugate. The variable substitution is then achieved through the relationships between structure factors (called power sums in algebra) and elementary symmetric polynomials, otherwise known as Newton's identities. The Newton's identities can be expressed in a recursive form:

$$(-1)^h F_h = \sum_{k=1}^{h-1} (-1)^{k-1} e_{h-k} F_k - h e_h \tag{A4}$$

The expressions for intensities I_h (h = 1, 2, …, N-1) in terms of the elementary symmetric polynomials (A2) can now be readily obtained as a product of F_h given by equation (A4) applied recursively by its complex conjugate given by the same equation where each e_h is replaced by e_{N-h} according to equation (A3). For example, the first three intensities are:

$$I_1 = e_1 e_{N-1}$$

$$I_2 = \left(e_1^2 - 2e_2\right)\left(e_{N-1}^2 - 2e_{N-2}\right) \tag{A5}$$

$$I_3 = \left(e_1^3 - 3e_1 e_2 + 3e_3\right)\left(e_{N-1}^3 - 3e_{N-1} e_{N-2} + 3e_{N-3}\right) \text{ , etc}$$

The first N-1 equations for $I_1,\ldots,I_{N-1}$ constitute the minimum lowest-degree system of polynomial equations with N-1 unknowns $e_1,\ldots,e_{N-1}$ sufficient for determination of the N-atom structure. Each set of e_h (h = 1, 2, …, N-1) determined by solving this polynomial system yields one structure, i.e. one set of the N atomic coordinates, as the N roots of the following univariate polynomial equation, by the mulivariate version of the Vieta's theorem:

$$\sum_{k=0}^{N} (-1)^{N-k} e_{N-k} \xi^k = 0 \quad , \tag{A6}$$

where $e_0 = 1$.

In summary, we demonstrated that all one-dimensional crystal structures consistent with the minimum set of N-1 intensities can be obtained by solving system of N-1 equations (A5) and then for each of its solutions ($e_1,\ldots,e_{N-1}$) solving a univariate polynomial equation (A6). Univariate polynomial equations can be solved by a robust algorithm (Aberth, 1973; Ehrlich, 1967; Bini, 1996), whereas a generally high-order polynomial system of many equations like system (A5) is a very difficult problem of modern algebra that requires investigation in each case. Prerequisite to solving system (A5) is an analysis of the number of its solutions, or crystal structures, that can be obtained from the N-1 intensities, as described in Section 2.2 of the main text.

Appendix B

Newton polytopes and the Bernstein's theorem on the number of roots of polynomial systems

This Appendix contains the algebraic terminology and the Bernstein's theorem used in the main text.

A Laurent polynomial is a function of N independent complex variables $\eta_1,\ldots,\eta_N$ defined as a sum of monomial terms $a_k\eta_1^{\beta_{1,k}}\ldots\eta_N^{\beta_{N,k}}$, where a_k are complex coefficients and $\beta_{1,k},\ldots,\beta_{N,k}$ are integer powers, which can be positive, zero or negative. This means that for each monomial there is one point in Euclidian space $\boldsymbol{R}^N$ whose coordinates are ($\beta_{1,k}$, …, $\beta_{\mathrm{N},k}$). For a given Laurent polynomial, these points define vertices of a polytope in $\boldsymbol{R}^N$. The convex hull of this polytope is called the Newton polytope of this polynomial. (A geometrical object is convex when a line segment between any two points that belong to this object lies entirely in that object. A convex hull of a polytope is a minimal convex polytope that contains the given polytope.) The

Minkowski sum of two polytopes A and B is a polytope, whose vertices are defined by vector sums of each vertex of polytope A and each vertex of polytope B.

The Bernstein's theorem states that a system of d Laurent polynomial equations with d unknowns has at most the number of roots equal to the so-called mixed volume of this system, V_{mix}, defined by the following linear combination of d-dimensional volumes $V_{M,p}$:

$$V_{mix} = \sum_{p=1}^{d} (-1)^{d-p} V_{M,p} \tag{B1}$$

where for a given p, $V_{M,p}$ are volumes of convex hulls of the Minkowski sums of all combinations of p different Newton polytopes of this system. For example, for a system of 3 polynomial equations with 3 unknowns:

$$V_{mix} = V(\text{conv}(A_1 + A_2 + A_3)) - V(\text{conv}(A_1 + A_2)) - V(\text{conv}(A_1 + A_3)) - V(\text{conv}(A_2 + A_3)) + V(A_1) + V(A_2) + V(A_3)\,, \tag{B2}$$

where A_k is the Newton polytope of the k-th polynomial in the system, the "+" symbol applied to the polytopes denotes their Minkowski addition, "conv" is the convex hull operator.

In practical cases where monomial coefficients are sufficiently generic (*e.g.* the monomial terms do not cancel out and the polynomials are not linearly dependent), the above mixed volume is known to be equal to the number of roots of the polynomial system. Therefore, the Bernstein's theorem provides a general approach to analyzing the number of roots of a multivariate polynomial system of d equations with d unknowns when variable elimination is not possible.

Appendix C

Properties of *h*-polytopes

In the main text, an M-dimensional h-polytope is defined by its $M(M+1)$ vertices: $2M$ vertices with one of their M coordinates equal to either h or $-h$ and the others equal to 0 and $M(M-1)$ vertices with two of their M coordinates equal to h and $-h$ and the others equal to 0. Examples of h-polytopes are given in Fig. 2 in the main text. Here, we will prove three remarkable properties of h-polytopes.

First, an M-dimensional h-polytope is a centrosymmetric convex hull. This follows from the fact that the h-polytope can be formed by cutting off parts of the hypercube (a convex hull) centered at the origin with the edge length of $2h$, by M-1 dimensional hyperplanes. This cutting procedure yields the $M(M+1)$ vertices of the h-polytope. This follows from the observation that the facets of the hypercube are cut so that each facet is defined by M vertices, a minimum needed to specify a facet. The coordinates of these M vertices for one facet all contain h or $-h$ for one of the M dimensions. In the other M-1 dimensions, the coordinates of the vertices are either contain all zeros, or contain $-h$ or h, respectively, thus describing the M vertices. We conclude the proof by noting that each of the vertices of the h-polytope is accounted for as a vertex of one of these facets. An h-polytope is centrocymmetric with the center of symmetry at the coordinate origin, because its vertex set is centrosymmetric.

Second, the convex hull of the Minkowski sum of an h_1-polytope and an h_2-polytope is an (h_1+h_2)-polytope. We proved above that these three polytopes are convex hulls. Note that the Minkowski sum contains the vertices of an (h_1+h_2)-polytope by construction. Therefore, owing to the convexity of an (h_1+h_2)-polytope, in order to prove the original statement it is sufficient to demonstrate that the rest of the points in the Minkowski sum belong to the (h_1+h_2)-polytope, i.e lie inside of it, or on its facets or edges. It can be demonstrated that each of the Minkowski sum points either lies on a line connecting two of the vertices of the (h_1+h_2)-polytope or on a line connecting the origin with one of its vertices. For the sake of brevity, we will illustrate this proof for some of the points. The coordinate origin belongs to this sum and lies in the (h_1+h_2)-polytope due to its centrosymmetry. The vertices of the h_1- and the h_2-polytopes belong to the (h_1+h_2)-polytope as they lie on the lines connecting the origin with the vertices of the (h_1+h_2)-polytope whose respective non-zero coordinates are at the same positions and have the same sign. Some of the sum points have coordinates that are equal to h_1 and h_2 at positions i_1 and i_2, respectively, to -h_1 and –h_2 at positions j_1 and j_2, respectively, and to 0 at the other M-4 positions. A point of this type lies on the line between two vertices of an (h_1+h_2)-polytope, one vertex with the i_1-th coordinate equal to h_1+h_2, the j_1-th coordinate equal to -h_1-h_2 and with the rest of the coordinates equal to zero and the other vertex with the i_2-th coordinate equal to h_1+h_2, the j_2-th coordinate equal to –h_1-h_2 and the rest of the coordinates equal to zero. Therefore, owing to the convexity of an (h_1+h_2)-polytope, such points belong to this polytope. Another set of Minkowski sum points have coordinates equal to h_1+h_2, -h_1 and -h_2 at positions i_1, i_2 and i_3, respectively and 0 at the other positions. These points lie on the line connecting a vertex with coordinates equal to h_1+h_2 and -h_1-h_2 at positions i1 and i2, respectively, and 0 at the rest of the positions and a vertex with the coordinates to h_1+h_2 and -h_1-h_2 at positions i_1 and i_3, respectively, and 0 at the rest of the positions. An analogous rationale applies to the Minkowski sum points whose three non-zero coordinates are equal to -h_1-h_2, h_1, h_2. The proof proceeds similarly for the rest of the points of the Minkowski sum.

Third, the volume of an M-dimensional h-polytope is equal to $h^M(2M)!/(M!)^3$ (equation (5) in the main text). The M coordinate axes and the origin divide the M dimensional space into

2^M hyperquadrants, each bounded by M-1 half-axes, either positive or negative, converging at the origin. The intersections of the h-polytope with these quadrants divide the polytope into non-overlapping objects whose total volume is the volume of the h-polytope. We will consider a hyperquadrant in which m coordinates are positive and M-m coordinates are negative. Now we will consider an intersection of an m-dimensional sub-space of this hyperquadrant in which the former m coordinates are positive and the other coordinates are zero with the h-polytope. Because no two coordinates of any vertex of the h-polytope are simultaneously positive, this intersection is formed by the origin and the m vertices lying on the respective axis at a distance h from the origin. This object is an m-dimensional pyramid (hyperpyramid) whose m-dimensional volume is equal to $h^m / m!$. By analogy, the (M-m)-dimensional volume of the intersection of the h-polytope with the space in which the other M-m coordinates are negative is equal to $h^{M-m} / (M-m)!$. Because for each of the former m positive directions and each of the latter M-m negative directions there is a vertex of the h-polytope whose respective coordinates are equal to h and $-h$ and the rest of the coordinates are equal to 0, the intersection of the original hyperquadrant with the h-polytope is a Cartesian product of the two hyperpyramids. The volume v of the intersection is then equal to the product of the two hyperpyramid volumes:

$$v = \frac{h^M}{m!(M-m)!} \tag{C1}$$

The number of such intersections is equal to the number of m-combinations in the set of M axes, i.e. $M!/(m!(M-m)!)$. Now, the volume of the h-polytope is obtained by summation over all intersection volumes:

$$V_{M,h} = h^M \sum_{m=0}^{M} \frac{M!}{[m!(M-m)!]^2} = \frac{h^M}{M!} \sum_{m=0}^{M} \left[\frac{M!}{[m!(M-m)!]} \right]^2 . \tag{C2}$$

The last sum in equation (C2) can be written in the closed form by using the Chu-Vandermonde identity to yield the initial expression:

$$V_{M,h} = \frac{h^M}{M!}\frac{(2M)!}{(M!)^2} = h^M \frac{(2M)!}{(M!)^3} \tag{C3}$$

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