Molecular Crystal Global Phase Diagrams: II. Reference Lattices

by R. B. McClurg and J. B. Keith

Notes to Accompany

Table 6: Structure Classification

Sphere Packing

See MEZDIE01 on pages 14 and 15. Notes refer to the hand-written letters on the following pages.

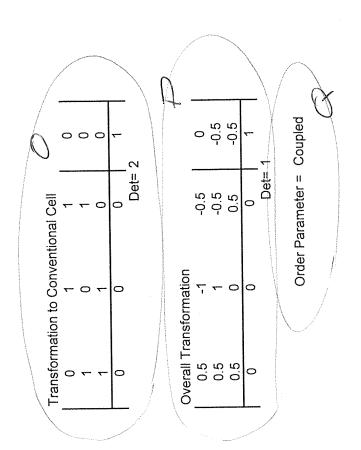
- A. CSD entry MEZDIE01 is described using space group 2 with a single molecule in the asymmetric unit with center of mass located at the Wyckoff site i. The Hermann-Mauguin label (P_-1) is provided for convenience.
- B. Unit cell parameters from MEZDIE01.cif
- C. Non-dimensional unit cell parameters using the a-axis length as the reference length
- D. Notes based on the neighbor histogram (separate document) indicating that there are 6 nearly equi-distant neighbors that are not in a single hemisphere. Therefore the structure appears to approximate a sphere packing. The remainder of the entry serves to classify the packing.
- E. Matrix representation for the parameters in C above. Euclidean norms of the columns give the desired magnitudes (1, 1.4527186, and 0.9209443). Dot products of the columns yield the product of the column norms and the cosine of the included angle according to the cosine law. The angles have the expected values (90.47694, 111.67244, and 89.98776 degrees). See Appendix A, equation 1.
- F. There is a single molecule in the asymmetric unit at Wyckoff site "i" with point symmetry "1".
- G. The fractional center-of-mass coordinates are provided for both molecules in the unit cell. See Appendix A, equations 2 and 3.
- H. A transformation matrix is provided which halves the volume of the unit cell (Determinant = ½), rotates the unit cell, and shifts the origin. Halving the volume of the cell recognizes that the center-of-mass lattice has a single molecule in the primitive unit cell. [The observed unit cell has two molecules in the unit cell due to orientation of the non-spherical molecules and minor translations of their centers.] See Appendix A, equations 4, 5, 7, and 8.
- I. The inverse transformation matrix is calculated for use below.
- J. The dot product of the matrix representation (E above) and the upper-left transformation submatrix (H above) yields the transformed matrix representation. See Appendix A, equation 6. Unit cell parameters are calculated using Euclidean norms and the cosine law as described in E above.
- K. The Niggli matrix, normalized using the (new) a-axis length is provided.
- L. The Niggli matrix conforms to the "Main Conditions" for a Type II reduced unit cell. Comparing the Niggli matrix to tabulated character definitions reveals that the reduced cell is triclinic (character 44), but close to body-centered-cubic (cI, character 5).
- M. Transforming the fractional center-of-mass coordinates (G) using the inverse transformation matrix (I) as indicated in the Appendix, equations 9 and 10, yields the indicated coordinates. Both molecules are near the origin (0,0,0) of a unit cell (modulo unity). This is a necessary condition for successful unit cell volume reduction (H). There is one molecule in the reduced unit cell (Z'=1). See Appendix A, equations 9 and 10.
- N. The observed unit cell (MEZDIE01), called the daughter, was observed in a space group with two symmetry operations (|G|=2) and two molecules per primitive unit cell (Z=2) yielding a symmetry density of one (|G|/Z=1). The identified BCC reference lattice

(space group 229) has 48 symmetry operations per primitive unit cell (|G|=48) and one molecule per primitive unit cell (Z'=1 as indicated in M above). The ratio yields a symmetry density of 48 for the BCC reference lattice. The ratios of the Z values gives the "size" and ratios of the symmetry densities gives the "index" of the symmetry-breaking transformation in passing from the reference lattice to the daughter cell. Note that the ratios are in opposite senses.

- O. The transformation from the reduced basis for character 5 to the conventional basis is tabulated along with the character definitions. See Appendix A, equations 11, 12, and 14.
- P. The matrix inverse of the product of the transformation matrices (H and O) yields the overall transformation matrix from the reference lattice (BCC) to the observed structure. The determinant of the transformation is unity since the conventional BCC reference cell and MEZDIE01 each contain two molecules. See Appendix A, equations 15 and 16.
- Q. COPL indicates that the overall transformation matrix is consistent with the indicated symmetry-breaking transition with size 2 and index 48 as calculated in N above. The order parameter is coupled.

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Rod Packing

See MECKIO on page 10. Notes refer to the hand-written letters on the following pages.

- A-D. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has two nearest neighbors forming rods. The rods are shown to have p-42m rod symmetry and pack in a nearly hexagonal arrangement.
- E. The indicated matrix transformation is analogous to that for MEZDIE01 above. See Appendix B, equation 19.
- F. The molecular centers-of-mass reside at Wyckoff point e with point symmetry m. The fractional coordinates are provided. See Appendix B, equations 20 and 21.
- G. Four sites on the 3-fold rotation axes of the molecule are indicated. They are used to determine the rod symmetry below.
- H. The indicated transformation matrix puts the rod axis along the x-axis, makes the y- and z-axes perpendicular to the rod axis, and shifts the origin to the center-of-mass of a selected molecule. See Appendix B, equations 22 and 23.
- I. The inverse of the transformation matrix is provided for use in transforming fractional coordinates.
- J. The rod axis, rod origin, and adjustable parameter in H are extracted from H for convenience.
- K. A second transformation rotates the rod about its axis to place the rod in standard orientation and rescales the coordinates perpendicular to the rod axis to make them equal in magnitude. See Appendix B, equations 24 and 25.
- L. The unit cell matrix representation (E) transformed by H and K yield the matrix representation L. The unit cell is tetragonal by design.
- M. The center-of-mass of the reference molecule is at the origin by design. The three-fold axes of the molecule very closely follow the Wyckoff orbit f of a p-42m rod symmetry in the 2^{nd} setting.
- N. There is one molecule in the rod unit cell.
- O. The symmetry-breaking transformation from rods to the observed structure has size 2 and index 4. See the analogous note N for MEZDIE01 above.

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Planar Packing

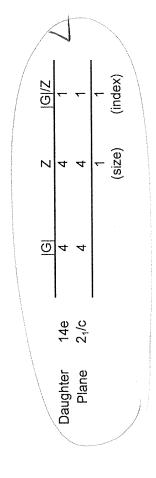
See CAMPOV on page 10. Notes refer to the hand-written letters on the following pages.

- A-E. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has three nearest neighbors forming two-dimensional planes. The planes are shown to have p2gg projection symmetry.
- F. The molecular centers-of-mass reside at Wyckoff point e with point symmetry 1. Fractional coordinates are provided.
- G. The indicated transformation matrix puts the plane into orthogonal axes. The inverse transformation is used to compute fractional center-of-mass coordinates in the transformed frame.
- H. No rotation nor any rescaling of axes are needed to put the plane into standard orientation.
- I. The matrix representation of the unit cell (E), after the indicated transformations (G and H), is an orthorhombic cell.
- J. Transforming the fractional center-of-mass coordinates (F) using the inverse transformation matrix (G) yields the coordinates indicated. There are four molecules in the primitive cell.
- K. The fractional coordinates (J) are consistent with p2gg projection symmetry (neglecting the z-coordinate) and $2_1/c$ symmetry when considering the third dimension.
- L. The symmetry-breaking transformation from planes to the observed structure has size 1 and index 1. See the analogous note N for MEZDIE above.

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Dimer Packing

See CARBTC on pages 10 and 11. Notes refer to the hand-written letters on the following pages.

- A-E. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has a single nearest neighbor. Therefore, the molecules form dimers with Cs point group symmetry.
- F. The molecular centers-of-mass reside at Wyckoff point e with point symmetry 1. Fractional coordinates are provided.
- G. The indicated transformation sorts the unit cell lengths in order to conform to reduced basis conventions. The inverse transformation is used to compute fractional center-of-mass coordinates in the transformed frame.
- H. The dot product of the matrix representation (E above) and the upper-left transformation submatrix (G above) yields the transformed matrix representation. Unit cell parameters are calculated using Euclidean norms and the cosine law.
- I. The Niggli matrix, normalized using the (new) a-axis length is provided.
- J. The Niggli matrix conforms to the "Main Conditions" for a Type II reduced unit cell. Comparing the Niggli matrix to tabulated character definitions reveals that the reduced cell is monoclinic (character 35), but close to C-centered-orthorhombic (oC, character 23).
- K. Transforming the fractional center-of-mass coordinates (F) using the inverse transformation matrix (G) yields the indicated coordinates. There are four distinct molecules in the primitive cell (Z'=4).
- L. Since cell reduction (G-K) did not yield a simpler reference lattice, and recognizing the single nearest neighbor, consider the centers-of-mass for dimers.
- M. The dimer centers-of-mass reside at Wyckoff point a with point symmetry -1. Fractional coordinates are provided.
- N. The indicated transformation halves the volume of the original unit cell (with matrix representation provided in E above) and rotates the unit cell. No origin shift is necessary in this case. Halving the volume of the cell recognizes that the center-of-mass lattice has a single dimer in the primitive unit cell.
- O. Applying the upper-left submatrix of the transformation to the original matrix representation yields the transformed matrix representation. Unit cell parameters are calculated using Euclidean norms and the cosine law.
- P. The Niggli matrix, normalized using the (new) a-axis length is provided.
- Q. The Niggli matrix conforms to the "Main Conditions" for a Type I reduced unit cell. Comparing the Niggli matrix to tabulated character definitions reveals that the reduced cell is C-centered monoclinic (character 10), but close to rhombohedral (hR, character 9).
- R. Transforming the fractional center-of-mass coordinates for the dimers (M) using the inverse transformation matrix (N) yields the indicated coordinates. There is one dimer in the primitive cell (Z'=1). The dimer center-of-mass is located at Wyckoff point a of rhombohedral space group R-3m (no 166).
- S. The symmetry-breaking transformation from the reference lattice containing orientationally disordered dimers to a monoclinic cell with disordered dimers has size one

- and index 3. Orientationally ordering the dimers is a subsequent transformation with size 4 and index 4.
- T. The tabulated transformation from a reduced basis in character 9 to the conventional cell (using the hexagonal setting for the rhombohedral cell) is indicated.
- U. The transformation from the reference lattice to the observed cell is given by the inverse of the product of the transformations in N and T above. This overall transformation matrix is provided. COPL indicates that the overall transformation matrix is consistent with the indicated symmetry-breaking transition with order parameter F2+.

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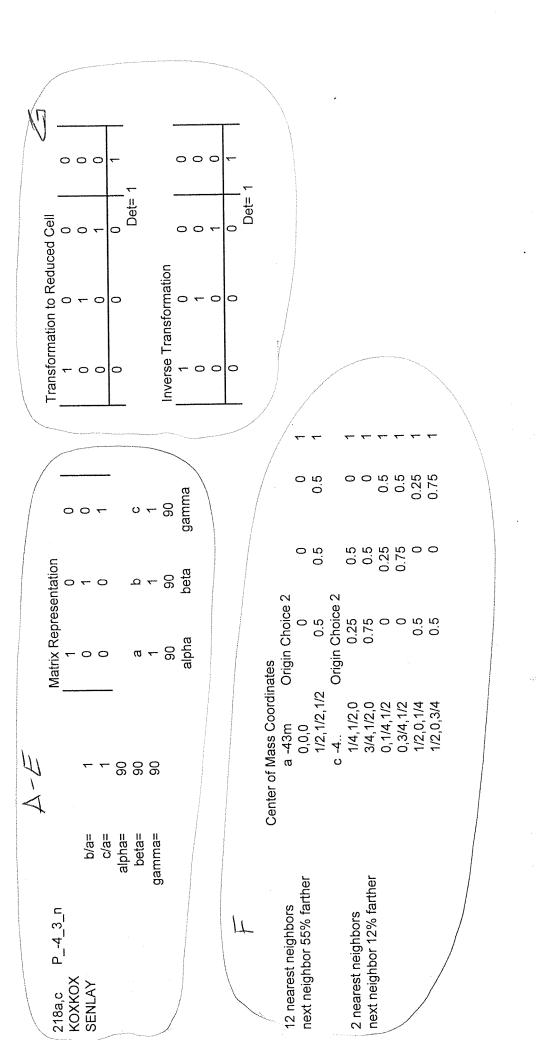
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Mixed Packing

See KOXKOX and SENLAY on page 1. Notes refer to the hand-written letters on the following pages.

- A-E. See corresponding notes for MEZDIE01. For this structure, the histogram indicates that each molecule has three nearest neighbors forming two-dimensional planes. The planes are shown to have p2gg projection symmetry.
- F. Two molecules in the unit cell reside at Wyckoff point a with point symmetry -43m. These molecules have 12 nearest neighbors. The remaining six molecules in the unit cell reside at Wyckoff point c with point symmetry -4. They have 2 nearest neighbors. Fractional coordinates are provided.
- G. Since the unit cell is already a reduced basis, there is no need for an additional transformation. The Identity matrix leaves the cell and the center-of-mass coordinates unchanged.
- H. The cell is a cube which belongs to primitive cubic (cP) character 3.
- I. The center-of-mass coordinates are consistent with Wyckoff orbits a and c of space group 223. In this case, the reference lattice has a higher symmetry than the observed structure solely due to the orientations of the molecules. There is no deformation of the cell nor translation of the centers-of-mass within the cell.
- J. The symmetry breaking transition in passing from the reference lattice to the observed (daughter) cell has size 1 and index 2.
- K. There is no transformation needed for character 3.
- L. The overall transformation matrix from observed cell to conventional reference lattice is the identity since the component transformations (G and K) are identities. COPL indicates that the overall transformation matrix is consistent with the indicated symmetry-breaking transition with size 1 and index 2 as calculated in J above. The order parameter is at the gamma point of the Brillioun zone (GM2-).



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