Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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Abstract

In the first part of this series (Keith *et al.*, 2004; Mettes *et al.*, 2004), we developed a method for constructing global phase diagrams (GPDs) for molecular crystals in which crystal structure is presented as a function of intermolecular potential parameters. In that work, a FCC center of mass lattice was arbitrarily adopted as a reference state. In part two of the series, we classify experimental crystal structures composed of tetrahedral point group molecules to determine what fraction of structures are amenable to inclusion in the GPDs and the number of reference lattices necessary to span the observed structures. We find that 60% of crystal structures composed of molecules with Td point group symmetry are amenable and that eight reference lattices are sufficient to span the observed structures. Similar results are expected for other cubic point groups.

1. Introduction

In the first part of this series, a method for constructing a global phase diagram (GPD) for molecular crystals of molecules of a given point group symmetry was developed (Mettes *et al.*, 2004). Conventional phase diagrams present the equilibrium phase behavior of a chemical substance or of a mixture of substances as functions of thermodynamic variables such as temperature, pressure, or composition. Global phase diagrams also present equilibrium phase behavior, but at least one of the independent variables of the diagram is either a parameter in an empirical equation of state or a parameter in an intermolecular potential. The classic example of a GPD of the first type is the classification scheme for high pressure vapor liquid phase equilibria by van Konyenburg (van Konyenburg & Scott, 1980). Their classification was based on the van der Waals equation of state with simple binary mixing rules. Despite the crude equation of state employed, it is still widely used to classify the phase behavior of real binary mixtures. Our GPDs are of the second type. They use an intermolecular potential constructed from a subset of a complete set of intermolecular potential basis functions for molecules sharing a particular point group symmetry. The parameters of the intermolecular potential are axes on GPDs. At the origin of each diagram is a plastic crystal phase that serves as the reference state for construction of the diagram. In the example developed previously, (Keith *et al.*, 2004; Mettes *et al.*, 2004) a diagram was constructed for molecules of T_d point group symmetry and a FCC reference lattice. These choices were motivated in part by the classic analysis of methane phase behavior (James & Keenan, 1959). Two independent variables were arbitrarily chosen in (Keith *et al.*, 2004) and three independent variables were chosen in (Mettes *et al.*, 2004).

Two issues were left unresolved in the previous contribution (Mettes *et al.*, 2004). First, the number and variety of reference lattices needed to summarize experimental

crystal structures was not determined. Although the FCC reference lattice is appropriate for cryogenic methane, it is expected that other reference lattices are required to span the diversity of observed crystal structures. Second, the number of independent variables necessary to span the diversity of intermolecular potentials was not determined. It has been asserted that too many parameters are needed to represent an intermolecular potential to be practical (Briels, 1980). This assertion was based on a particular method for associating a potential with a parameter set. While the method employed was reasonable, it is not the only possibility. It left open the possibility that another association would lead to a more practical parameter set dimensionality. The first issue is addressed in this contribution while the second is addressed in a separate contribution (Keith & McClurg, 2009).

The outline of the balance of the paper is as follows. In Sec. 2 we discuss the derivation of our data set, its chemical and crystallographic characteristics, and classify entries based on structural similarity. In Sec. 3 we deduce reference lattices for each structure. The resulting assignments and their implications for use in constructing Global Phase Diagrams are discussed in Sec. 4.

2. Data set

Since molecular crystal global phase diagrams are constructed for molecules of a given molecular point group symmetry, we have chosen to use the *CSDSymmetry* database as the primary source of crystal structures for this study (Yao *et al.*, 2002). This database summarizes the point groups of molecules that form non-disordered, non-polymeric, non-ionic, coordinate-determined molecular crystals in the CSD. Duplicate structures were removed from the database and hydrogen atoms were not considered when assigning point groups. While the methods introduced in our previous work (Mettes *et al.*, 2004) are applicable to disordered structures, which are sys-

tematically absent from *CSDSymmetry*, it is a convenient source of crystal data for molecules of a particular point group. Our methods are restricted to single component crystals, however. Therefore we worked with the single component crystal subset of the *CSDSymmetry* database. This was accomplished by first querying the CSD for all single component crystals using CONQUEST, the interface to the CSD, and then using CONQUEST to take the intersection of the two data sets.

Continuing the example begun in our prior work (Mettes *et al.*, 2004), we chose to consider crystals composed of molecules with T_d molecular point group symmetry. We have augmented the data from *CSDSymmetry* with a recently determined structure of the low temperature ordered phase of heavy methane (Neumann *et al.*, 2003). The data set contains 71 crystal structures of 70 different chemical substances. Only carbon tetrachloride (CCl_4) appeared twice in different polymorphs. [CSD structures CARBTC (Piermarini & Braun, 1973) and CARBTC07 (Cohen *et al.*, 1979)]. Names and chemical formulas for all the entries are given in (supplementary) Table 9 available from the publisher. The chemical structures include 15 hydrocarbons and their substituted derivatives and 56 organometallics. The organometallics contain 30 different metals: Al, As, Bi, Cd, Co, Cs, Cu, Ga, Ge, Hf, In, Mg, Mn, Na, Ni, Np, Pb, Pt, Re, Rh, Ru, Sb, Si, Se, Sn, Tc, Th, Ti, U, and Zn. Eight molecular framework types, also shown in (supplementary) Table 9, are present in the data set: Cubane (29), Adamantane (17), MX_4 (16), Tetrahedrane (3), and others (6). There are entries from all seven crystal systems in the data set. Twenty crystals are cubic (also called isometric), one is hexagonal, five are trigonal, ten are tetragonal, six are orthorhombic, twenty-two are monoclinic, and seven are triclinic (also called anorthic) as illustrated in Figure 1. This distribution is different than the CSD as a whole (Baur & Kassner, 1992), but that is not surprising given the larger-than-average number of symmetries in the T_d point group. The data set is sufficient however to test whether molecular crystal global

phase diagrams apply to organic and organometallic molecules, a variety of molecular frameworks, and all seven crystal systems.

2.1. Space Group Assignment Corrections

Several researchers have shown that structures with incorrect space group assignments account for at least 3% of the entries in the Cambridge Structural Database (CSD).(Baur & Tillmanns, 1986; Marsh, 1995) Given the size of the test set used in this study, it is to be expected that a few errors must be identified and corrected.

CSD entry JUFWUC (Tesh *et al.*, 1992) appears to have been incorrectly assigned to space group $P23$ (no. 195) rather than $P\bar{4}3m$ (no. 215). Both space groups are members of the generic cubic extinction symbol P - - -. Thus they have no systematic extinctions and thus x-ray diffraction peaks occur in all of the same positions for both groups. They belong to different Laue classes however. Space group 195 is in Laue class $m\bar{3}$ while space group 217 is in $m\bar{3}m$. Space group 195 is a subgroup of 215 of order two. The symmetry operation present in 215, but missing in 195 is a face-diagonal mirror plane. The fractional coordinates for the Cs, N, and Si atoms provided by the authors are all consistent with the existence of the "missing" mirror plane. The fractional coordinates of the carbon atoms are very nearly consistent with the existence of the mirror plane and are within the indicated error given by the authors. The hydrogen atom positions provided in JUFWUC.cif were calculated and not determined experimentally. Therefore they do not provide independent evidence of the crystal symmetry. Evidently the structure was determined under space group 195, but space group 215 cannot be ruled out based on the authors own estimates of the uncertainties in the fractional coordinates. It is standard practice to accept the higher symmetry space group in this case.

CSD entry HMGETP (Dahl *et al.*, 1976) appears to have been incorrectly assigned

to space group $I23$ (no. 197) rather than $I\bar{4}3m$ (no. 217). Both space groups are members of the generic body-centered cubic extinction symbol I---. Thus they have the same systematic extinctions and thus x-ray diffraction peaks occur in all of the same positions for both groups. They belong to different Laue groups however. Space group 197 is in Laue class $m\bar{3}$ while space group 217 is in $m\bar{3}m$. Space group 197 is a subgroup of 217 of order two. The symmetry operation present in 217, but missing in 197 is a face-diagonal mirror plane. The fractional coordinates for the Ge and P atoms provided by the authors are all consistent with the existence of the "missing" mirror plane. The fractional coordinates of the carbon atoms are very nearly consistent with the existence of the mirror plane. Since no error estimate for the fractional coordinates was provided by the authors, the distance from the given atomic position to the proposed mirror plane was calculated as an indication of the difference between the reported symmetry and the proposed symmetry. Adjusting the carbon atom positions by 0.0049Å along two coordinate directions restores the "missing" mirror plane. This is well within the resolution of the structure determination. No hydrogen atom positions were provided in HMGETP.cif. Evidently the structure was determined under space group 197, but space group 217 cannot be ruled out based on a reasonable estimate of the uncertainties in the fractional coordinates. It is standard practice to accept the higher symmetry space group in this case.

It is interesting to note that both of the above structures appear to have been mistakenly assigned to a lower-than-necessary space group due to the omission of a face-diagonal mirror plane. Assignment of the structure to the incorrect space group is due to the incorrect Laue point group assignment. This is a type 2 error in the nomenclature of Baur and Tillmanns (Baur & Tillmanns, 1986). In such cases, the reported structure is very similar to the presumed correct structure. Correcting the error requires only adjusting the reported atomic fractional coordinates and changing

the reported space group.

One entry [CSD structure XUWROW (Sung *et al.*, 2002)] is a very unusual structure containing 70% voids as recorded by the CCDC staff in the corresponding cif file in the CSD. Although low density sphere packings are possible, stability requires that each sphere be surrounded by at least four neighbors that are not in the same hemisphere (Conway & Sloane, 1998). Structure XUWROW has large voids separating layers of molecules parallel to the {001} plane. Molecules at the edges of the layers have all of their neighbors in a single hemisphere and therefore violate a necessary condition for sphere packing stability. Also, the layers are separated by wide voids in the reported structure. Dispersion interactions between the layers would tend to narrow these wide void layers. For these reasons, it seems likely that the reported crystal structure is mechanically unstable. According to the original publication, the crystal was grown as a thin epitaxial crystal under ultra-high vacuum. Apparently the crystal structure is either strongly influenced by the substrate which stabilizes the crystal or the structure was not determined correctly. In either case, it is not an independent stable form we therefore exclude it from further consideration.

3. Classification

Neglecting CSD structure XUWROW and reassigning structures JUFWUC and HMGETP as discussed above, the remaining crystal structures were organized into groups that bear a strong "structural relation" as discussed in the first edition of Volume C of the International Tables for Crystallography (ITC) (Hahn, 1983). For crystals to belong to the same group they must have the same space group symmetry, cell lengths in similar proportions, similar cell angles, and molecular centers at equivalent Wyckoff point(s) with similar structural parameter values where applicable. Crystal structures with alternative origin and/or cell choices were transformed to consistent cell and ori-

gin choices prior to assessing their structural relationship, if any. For monoclinic space groups, cell choice 1 with unique axis b was utilized. For Rhombohedral space groups, the obverse setting of the hexagonal cell was utilized. Origin choice 2 was utilized in cases where more than one origin is provided in the International Tables for Crystallography. For molecules located at Wyckoff points that belong to an equivalent set, preference was given to the label occurring first alphabetically. Thus, Wyckoff point a was selected rather than b in space group $P\bar{4}2_1c$ (no. 114) since both are equivalent. We refer to the members of these structurally related groups as sharing a distinct structure. Note that we do not require that the atomic positions be similar to be classified in the same distinct structure. For example, two structures [CSD structures DILWIE01 (Ebert *et al.*, 1998) and ZEYHIU (Noth & Thomann, 1995)] crystallize in space group $P\bar{3}c1$ (no. 165) with molecular centers at Wyckoff point d. Their cell parameters are also in similar ratios. Therefore, we classify them in the same distinct structure, despite their different chemical structures with different numbers of atoms.

The 70 crystal structures fall into 46 distinct structures. Five structures are cubic (*aka* isometric), one is hexagonal, four are trigonal, eight are tetragonal, six are orthorhombic, sixteen are monoclinic, and six are triclinic (*aka* anorthic). These distinct structures are further characterized based on the number and relative positions of neighboring centers-of-mass in the following subsections. The center-of-mass lattice is used here to be consistent with the reference state employed in the prior work (Keith *et al.*, 2004; Mettes *et al.*, 2004). In the fully orientationally disordered reference state only the center-of-mass distances are relevant. As the temperature is reduced, the systems undergo symmetry-breaking phase transitions through orientation of the constituent molecules. For the oriented molecules the closest contacts and/or the strongest interactions may be with molecules that are not nearest neighbors with respect to centers-of-mass. The interactions are addressed in (Keith *et al.*, 2004; Mettes

et al., 2004) while this work focuses solely on the assignment of the reference lattice.

3.1. Sphere Packings

In 42 structures there are four or more neighbors that are equidistant or nearly equidistant. Also, the neighbors are not all in one hemisphere relative to the (arbitrary) reference molecule. Such structures are identified as sphere packings (Conway & Sloane, 1998), and classified by the space group symmetry of the center-of-mass lattice. The center-of-mass lattice is called the reference lattice for brevity and for consistency with our prior work (Keith *et al.*, 2004; Mettes *et al.*, 2004). The structures and their reference lattices are tabulated in Table 1.

For 15 crystal structures, assignment of the reference lattice is trivial since the unit cell shares the same Bravais symmetry as the reference lattice and the molecules sit at high symmetry locations in the crystal. This is true of the structures in space groups $Fd\bar{3}m$ (no. 227), $I\bar{4}3m$ (no. 217), and $P\bar{4}3m$ (no. 215) with Diamond Cubic, Body-Centered Cubic, and Simple Cubic reference lattices, respectively.

The body-centered cubic space group $I\bar{4}3m$ (no. 217) with molecules at Wyckoff point a is the most common structure in the data set with 11 different crystal structures. The CSD structure labeled NIWMIP is used as an example of that structure in Figure 2. The vertical axis in the figure is the symmetry density defined as the ratio of the order of the symmetry group to the number of molecules. Along the horizontal axis are insets showing the molecular structure on the left, the reference lattice on the right, and the crystal structure in the middle. The diagram shows symmetry breaking during creation of the crystal. For a symmetry breaking, the ratio of the symmetry density prior to and after the transitions gives the index of the transition. To facilitate visual comparisons of transition indices, the symmetry density is plotted on a logarithmic scale in the figures. Figure 2 conveys that the full molecular symmetry is

retained while the BCC reference lattice symmetry is broken in forming the structure in space group 217. The broken symmetry is the inversion which yields an index of two.

The four crystal structures assigned to the HCP reference lattice are all slightly compressed along the c-axis relative to the expectation for ideal close-packing of spheres. This is consistent with the observation for many other HCP structures (Sands, 1993). Of the elements that adopt HCP structures, only helium adopts the ideal unit cell dimension ratio, $c/a = (8/3)^{1/2}$. Cadmium and zinc adopt elongated unit cells with $c/a > (8/3)^{1/2}$. Twenty two other elemental solids adopt slightly compressed HCP structures with $c/a < (8/3)^{1/2}$. Despite variation in the unit cell dimension ratios, these elements are commonly described as adopting the HCP crystal structure. We utilize the same flexibility in nomenclature when assigning the HCP reference lattices to molecular solids.

For 23 crystal structures, symmetry breaking in passing from the reference lattice to the observed structure leads to dramatic changes in the conventional unit cell size and/or shape. Reference lattice assignment in these cases is not trivial. The CSD structure labeled MEZDIE01 serves to illustrate the process. MEZDIE01 has a triclinic unit cell in space group $P\bar{1}$ (no. 2) with molecular centers at the general Wyckoff point i. The alpha and gamma angles of the unit cell are very close to 90 degrees, so that the unit cell is metrically similar to a monoclinic cell, but the connection to a BCC reference lattice is not immediately evident. The fractional coordinates of the molecular centers-of-mass are very close to one-quarter and three-quarters of the distance along a cell body diagonal. If the molecular centers were at precisely these locations, and molecular orientational ordering is ignored, then the unit cell of the reference lattice can be halved in volume using a matrix transformation. The resulting unit cell has one molecular center per reduced cell. The reduced cell is nearly equi-axed

(cell lengths differ from the mean by less than 1%) and nearly rhombohedral (angles differ from the mean by less than 1 degree). The reduced cell belongs to character number 44 (triclinic), but is only slightly distorted from character 5 (BCC). Applying the standard matrix transformation (for character 5) from the reduced cell to the conventional cell yields the reference lattice. The product of the two matrix transformations gives the overall transformation from the reference lattice to the observed crystal structure. Finally, the overall transformation matrix is confirmed using COPL (Stokes *et al.*, 2007). COPL confirms that all of the symmetry elements present in the daughter structure are inherited from the reference lattice, confirms the index of the transformation, and provides the complete order parameter list for the transformation. The matrix unit cell representations and matrix transformations used in determining the reference lattice assignment starting with MEZDIE01 are given in an Appendix. The same information for each of the structures identified with sphere packing reference lattices and their associated COPL outputs are summarized in (supplementary) Table 8.

Six crystal structures were identified with the diamond reference lattice. Only one of these, ZNOXAC01, retains the cubic unit cell with four nearest neighbors for each molecular center. The other five are significantly distorted. Two are compressed, one is elongated, and two are orthorhombically distorted similar to the γ-Plutonium structure with ten equidistant neighbors (NRL, 2009). These distortions may be due to the low packing density of the ideal diamond cubic lattice relative to the other reference lattices.

3.2. Rod Packings

In 16 crystal structures there are two neighbors that are equidistant or nearly equidistant and the third neighbor is significantly further away than the second. In an

additional six crystal structures, there are three or four equidistant or nearly equidistant neighbors, but these neighbors are all in a single hemisphere. For all 16 crystal structures, a synthon based on one-dimensional chains of molecules have been identified. Here the term synthon is used to refer to substructures present in crystal structures. A similar concept is described by Lauher (Lauher, 2004) and called networks. Chains of molecules are classified by their rod symmetries (Hahn, 2002*a*). Classification of the structures in these cases requires identification of the rod symmetry and the lateral packing motif.

The CSD structure labeled MECKIO is used as an example of a crystal structure composed of rods. Its symmetry breaking plot is illustrated in Figure 4. The inset on the left is an isolated monomer with Td symmetry (G/Z=24/1). Second from the left is a rod packing with rod group $p\bar{4}m2$ (G/Z=8/1). The inset on the far right is a two-dimensional hexagonal packing representing the lateral packing of the rods (G/Z=12/1). Second from the right is the crystal structure with one rod emphasized for clarity (G/Z=4/2). The crystal is viewed end-on to emphasize nearly hexagonal packing of rods. The symmetry density decreases at each stage of building the crystal from its constituents.

All of the crystal structures composed of laterally packed rods are summarized in Table 2. In the subset of crystal structures containing rod packings, five different rod symmetries were identified, $pmcm$ (7/16, 44%), $p\bar{4}m2$ (4/16, 25%), $p\bar{1}$ (4/16, 25%), and $pc11$ (1/16, 6%). The majority of the rods packed laterally in hexagonal close-packing (9/16, 56%) while a significant fraction adopted a square packing (6/16, 38%), and only one example of a decidedly oblique packing (1/16, 6%) was observed. A total of eight combinations of rod symmetries and lateral packings were observed.

In the CSD structure labeled RIMNAC the rods have $p\bar{4}m2$ symmetry and adopt a nearly hexagonal lateral packing, but there are three independent rotations about

the rod axis. These three rotations lead to three independent Wyckoff orbits. This is in contrast to most of the other structures in the data set for which the orientations of the rods are related by symmetry operations of the three-dimensional crystal.

3.3. Planar Packings

In five structures there are three or four neighbors that are equidistant or nearly equidistant and the next neighbor is significantly further away than the second. Also, the neighbors are either coplanar or in one hemisphere relative to the (arbitrary) reference molecule. Such structures are identified as planar packings, and classified by their planar group symmetry (Hahn, 2002*a*). The structures and their planar group symmetries are tabulated in Table 3.

The CSD structure labeled MZNMOX10 is used as an example of a crystal structure composed of planes of molecules. Its symmetry breaking plot is illustrated in Figure 5. The inset on the left is an isolated monomer with Td symmetry (G/Z=24/1). On the far right is a two-dimensional square packing representing the center-of-mass lattice in the plane (G/Z=8/1). Second from the right is a planar packing with point group $S4$ (G/Z=4/1). Because the molecules are tipped slightly in the three-dimensional crystal, the plane is not viewed along its normal in the inset, but is viewed along the molecular S4 axis to emphasize the symmetry of the undistorted planar packing. Second from the left is the crystal structure with one plane emphasized for clarity (G/Z=4/4=1). The vertical axis indicates that symmetries are broken at each stage.

3.4. Dimer Packings

In three structures there is one closest neighbor and the next closest neighbor is significantly further away than the first. Such structures are identified as dimer packings, and classified by their dimer point group symmetry. The structures and their

dimer point group symmetries are tabulated in Table 4.

FOJBUB02 and VADRAU are cubic structures in space group $Pa\bar{3}$ (no. 205) with molecules at Wyckoff point c, which has $C3$ point group symmetry. Their second nearest neighbors are 33% and 25% further than the closest, respectively. Therefore, we consider these dimers as the synthon for the crystal. The dimer centers of mass are at Wyckoff point a, with $C3i$ point group symmetry. The dimer centers of mass form a perfect face centered cubic lattice. The symmetry breaking plot for FOJBUB02 is given in Figure 6. The symmetries of the monomer and the FCC reference lattice are broken in creating the crystal, but the dimer symmetry is retained in the three-dimensional crystal.

LUFYEQ is a tetragonal structure in space group $I4_1/a$ (no. 88) with molecules at the general Wyckoff point, f. Since the second nearest neighbor is 33% further than the first, there are dimers serving as synthons for the crystal. The dimers reside at Wyckoff point e, with $C2$ point group symmetry. Each dimer has one neighboring dimer that is closer than any other. Therefore, the dimers pair to produce quadramers at Wyckoff point a, with $S4$ point group symmetry. The quadramer center of mass lattice is a somewhat compressed diamond cubic structure.

CARBTC is a fourth structure identified as a dimer packing, but this assignment is less apparent from the histogram of neighbor distances. In the structure, each molecule has one nearest neighbor and two additional neighbors that are 6% further. This is insufficient for a sphere packing and the arrangement of molecules is inconsistent with simple planar packings. Therefore, the packing was analyzed using dimers centered at an inversion of space group $P2_1/c$ (no. 14).

3.5. Mixed

Three crystal structures belonging to a common distinct structure do not fit in the above classification system because molecules residing at different Wyckoff positions have different numbers of nearest neighbors. Structures KOXKOX, SENLAY, and RUQMEV are cubic structures in space group $P\bar{4}3n$ (no. 218) with molecules at Wyckoff positions a and c. The structures are tabulated in Table 5. The molecules at Wyckoff position c form rods with rod group $p\bar{4}m2$ running parallel to all three orthogonal coordinate directions. The molecules at Wyckoff position a each have twelve equidistant nearest neighbors in a slightly distorted icosahedral coordination. Although there are other crystal structures with multiple Wyckoff orbits in the data set, these three structures differ because the coordination of nearest neighbors is qualitatively different for the two sets. In the other examples, the neighbor histograms are only subtly different when comparing the various orbits.

4. Discussion and Conclusions

Identification of lower-dimensionality synthons as a means of describing three-dimensional crystals has been discussed previously (Lauher, 2004). The crystal structures identified here as rod packings have been called α-networks and planar packings have been called β-networks in the nomenclature of (Lauher, 2004). The molecules used by Lauher to illustrate sub-periodic networks were polar and their intermolecular interactions had strong hydrogen bonding and/or ionic character. Formation of strongly bound one-dimensional structures is common, but not universal, in such cases. Two types of two-dimensional structures were identified by Lauher. The first is a two-dimensional synthon composed of parallel one-dimensional rods, called α-networks. The second is a fundamentally two-dimensional structure without α-network substructures. In all of his examples, three dimensional crystal structures were composed of one- or two-

dimensional networks.

Given the cubic point group symmetry (Td) of the molecules considered here, we expected that the corresponding crystal structures would be composed of molecules having multiple equidistant and isoenergetic interactions with four or more neighbors leading to sphere packings or γ-networks in Lauher's nomenclature. This expectation proved accurate for 60% (42/70) of the structures. Of these, BCC (16/42, 38%) and FCC (12/42, 29%) were the most common reference lattices. HCP and SC reference lattices contributed 10% (4/42) each. Only one structure (2%) adopted the ideal diamond cubic lattice, but five structures (12%) were identified with three grossly distorted diamond cubic structures. Together, these eight reference lattices span the observed diversity of crystal structures based on sphere packings and are illustrated in Figure 7 under the "Sphere Packing" trunk.

Somewhat unexpected was the 40% (32/70) of structures that adopted lower-dimensionality synthons. The next largest subset of the crystal structures were composed of rods. They comprised 23% (16/70) of the structures. A total of eight combinations of rod symmetries and lateral packings were observed.

Smaller fractions of other structures were assigned. Five cases (5/70, 7%) of planar structures, also called β-networks were observed. Four cases (3/70, 4%) of spherical packings of dimers and one case (1/70, 1%) of a spherical packing of quadramers were assigned. Finally, three isostructural examples (3/70, 4%) of a mixed sphere and rod packing in space group $P\bar{4}3n$ (no. 218) belonged to the data set. Given the small numbers of these structural types, their relative proportions may not be accurately determined in this set of data. Also, the possibility of unobserved structural motifs cannot be excluded. Figure 7 shows lower-dimensional and oligomer sythons under the "Other" trunk, which are further broken down to specialized types of rod packings and so on.

The goals of the research described in this report was to determine the frequency of sphere packings which are readily amenable to inclusion in the global phase diagrams (GPDs) developed previously (Keith *et al.*, 2004; Mettes *et al.*, 2004). In the set of crystal structures composed of molecules in the Td point group, 60% are amenable to inclusion in the global phase diagrams using the molecule as the synthon. Eight reference lattices span the diversity of observed center of mass lattices so that a set of at least eight global phase diagrams are required to represent the phase behavior of the sphere packing subset of the data set. Dimer and quadramer packing structures are also suitable for inclusion in GPDs using the point group symmetry of the synthon. These account for another 6% of the crystal structures. Similar proportions are expected for molecular symmetries belonging to other cubic point groups.

A qualitatively different set of phase diagrams are required for the structures that adopt lower-dimensionality synthons (rod and planar packings) or mixed structures. The presence of such structures implies a hierarchy of interaction strengths. We expect that strong interactions lead to the rods while weaker interactions are responsible for lateral packing of the rods into crystals. Such a hierarchy of interaction strengths is expected for molecules belonging to lower molecular point group symmetries. Therefore for non-cubic point group symmetries, it is expected that the proportion of crystal structures classified as sphere packings would be smaller and the proportion of rod and planar packings would be greater than that reported here for tetrahedral molecules.

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Appendix A
Sphere Packings

For 42 of the 70 crystal structures in the data set considered, the center of mass distribution was identified with a sphere packing. For 15 of these, the identification was trivial since the unit cell has the same symmetry as the idealized sphere packing. For the remaining 27 structures, the center of mass distribution is slightly distorted from the idealized sphere packing. The process of identifying the sphere packing is not trivial in these cases because unit cell distortions and/or translation of the centers of mass change the symmetry of the center of mass lattice. To illustrate the process of reference lattice assignment, the CSD structure MEZDIE01 is considered in detail below. Details of the reference lattice assignments for all 42 structures are summarized in (supplementary) Table 6 and accompanying notes available from the journal publisher.

CSD structure MEZDIE01 has a triclinic unit cell with $b/a = 1.4627$, $c/a = 0.9209$, $\alpha = 90.48\,\mathrm{deg}$, $\beta = 111.67\,\mathrm{deg}$, and $\gamma = 89.99\,\mathrm{deg}$. The unit parameters can be conveniently represented in matrix form where the matrix columns correspond to the cell vectors and the rows are components of the vectors parallel to orthonormal laboratory frame coordinates,

$$\mathbf{M}_1 = \begin{bmatrix} 1 & 0.0003 & -0.3401 \\ 0 & 1.4627 & -0.0076 \\ 0 & 0 & 0.8558 \end{bmatrix}. \qquad (1)$$

The molecular centers of mass are located at fractional coordinates, $x = 0.7606$, $y = 0.2506$, and $z = 0.2418$ and at the location related by inversion about the cell body center. Unit cell transformations are facilitated using four dimensional vectors

in which the fourth component is unity.

$$\boldsymbol{\nu}_1 = \begin{bmatrix} 0.7606 \\ 0.2506 \\ 0.2418 \\ 1 \end{bmatrix} \tag{2}$$

$$\boldsymbol{\nu}'_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 2 \end{bmatrix} - \boldsymbol{\nu}_1. \tag{3}$$

Enumeration of the neighboring centers of mass for an arbitrarily chosen reference molecule reveals that there are six neighbors within a shell 3% larger than the nearest neighbor distance and two additional neighbors within a shell 11% larger than the nearest neighbor distance. These neighboring molecular centers are neither coplanar nor are they all in a single hemisphere. Therefore, the molecular centers satisfy the conditions for a (slightly distorted) sphere packing reference lattice.

Recognizing that the molecular center fractional coordinates are nearly one-quarter and three-quarters of the distance along a body diagonal suggests that a matrix transformation with determinant equal to one-half is needed to generate the reduced cell for the reference lattice with one molecule per cell. The following matrix transformation suffices for the current example,

$$\mathbf{T}_{12} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & -1/2 & 0 \\ 1/2 & 1/2 & -1 \end{bmatrix} \tag{4}$$

$$|\mathbf{T}_{12}| = 1/2. \tag{5}$$

Such transformations may be generated by inspection of the neighbor coordinates relative to the chosen reference center or by using the LePage software as implemented in the CheckCell program, for example (CCP14, 2004).

The matrix representation of the reduced cell is given by the matrix product of the original matrix representation and the transformation matrix,

$$\mathbf{M}_1 \cdot \mathbf{T}_{12} = \begin{bmatrix} 0.3301 & 0.3298 & 0.3401 \\ 0.7276 & -0.7352 & 0.0076 \\ 0.4279 & 0.4279 & -0.8558 \end{bmatrix} \tag{6}$$

The reduced cell has $b/a = 1.0066$, $c/a = 1.0161$, $\alpha = 108.00\,\mathrm{deg}$, $\beta = 107.31\,\mathrm{deg}$, and $\gamma = 107.084\,\mathrm{deg}$. Construction of the Niggli matrix indicates that this triclinic cell (character 44) is reasonably close to the reduced cell corresponding to the body-centered cubic cell (character 5) (Hahn, 2002*b*). For the idealized character 5 reduced cell, $b/a = c/a = 1$ and $\alpha = \beta = \gamma = cos^{-1}(-1/3) \approx 109.47\,\mathrm{deg}$. For the experimental reduced cell, the angles are roughly two degrees smaller than the ideal value which indicates that the primary distortion is rhombohedral. Smaller perturbations lead to slightly unequal unit cell length and angle parameters.

To determine the fractional coordinates of the centers of mass in the transformed coordinates, it is convenient to define an augmented transformation matrix as follows,

$$\mathbf{S}_{12} = \begin{bmatrix} \mathbf{T}_{12} & \mathbf{w}_{12} \\ \mathbf{0} & \mathbf{1} \end{bmatrix} \tag{7}$$

where w_{12} is the origin shift in the original coordinate system. In this case,

$$\mathbf{w}_{12} = \begin{bmatrix} 3/4 \\ 1/4 \\ 1/4 \end{bmatrix}. \tag{8}$$

Then the transformed coordinates are given by

$$\boldsymbol{\nu}_2 = \mathbf{S}_{12}^{-1} \cdot \boldsymbol{\nu}_1 = \begin{bmatrix} 0.0112 \\ 0.0100 \\ 0.0188 \\ 1 \end{bmatrix} \tag{9}$$

$$\boldsymbol{\nu}'_2 = \mathbf{S}_{12}^{-1} \cdot \boldsymbol{\nu}'_1 = \begin{bmatrix} -0.0112 \\ -1.0100 \\ -1.0188 \\ 1 \end{bmatrix} \tag{10}$$

both of which are reasonably close to the origin, modulo integer translations of the unit cell.

Since the reduced cell is close to the character 5 conditions with one molecule close to the origin, the sphere packing is identified with the BCC reference lattice. Applying

the tabulated transformation of the reduced cell to the conventional cell, (Hahn, 2002*b*)

$$\mathbf{T}_{23} = \begin{bmatrix} 0.5 & -1 & -0.5 & 0 \\ 0.5 & 1 & -0.5 & -0.5 \\ 0.5 & 0 & 0.5 & -0.5 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{11}$$

$$|\mathbf{T}_{23}| = 2 \tag{12}$$

yields the matrix representation of the conventional unit cell,

$$\mathbf{M}_3 = \mathbf{M}_2 \cdot \mathbf{T}_{23} = \begin{bmatrix} 0.6699 & 0.6702 & 0.6599 \\ -0.7276 & 0.7352 & -0.0076 \\ -0.4279 & -0.4279 & 0.8558 \end{bmatrix}. \tag{13}$$

As anticipated above, the cell is slightly distorted from an ideal cubic cell, primarily by a rhobohedral distortion ($b/a = 1.005$, $c/a = 1.003$, $\alpha = 86.5\,\mathrm{deg}$, $\beta = 86.0\,\mathrm{deg}$, $\gamma = 85.2\,\mathrm{deg}$).

Since the center of mass is at the origin in both the reduced cell and the BCC reference lattice, there is no need for another origin shift and the augmented transformation matrix is

$$\mathbf{S}_{23} = \begin{bmatrix} \mathbf{T}_{23} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{bmatrix}. \tag{14}$$

The overall transformation from the reported crystal structure of MEZDIE01 to the BCC reference lattice is the matrix product of the stepwise transformations,

$$\mathbf{S} = \mathbf{S}_{12} \cdot \mathbf{S}_{23} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \tag{15}$$

$$|\mathbf{S}| = 1 \tag{16}$$

and the transformed coordinates are given by

$$\boldsymbol{\nu}_3 = \mathbf{S}^{-1} \cdot \boldsymbol{\nu}_1 = \begin{bmatrix} 0.0088 \\ 0.0100 \\ 0.0012 \\ 1 \end{bmatrix} \tag{17}$$

$$\boldsymbol{\nu}_3'' = \mathbf{S}^{-1} \cdot \left(\boldsymbol{\nu}_1 + \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right) = \begin{bmatrix} 0.5088 \\ 0.5100 \\ 0.5012 \\ 1 \end{bmatrix}. \tag{18}$$

The determinant of the overall transformation $|\mathbf{S}|$ is unity so that the volumes of the initial cell and the reference lattice cell are the same in this case. Both contain two molecules, but they are paired differently as reflected in the use of primes in the center of mass coordinates, $\boldsymbol{\nu}'_1$, $\boldsymbol{\nu}'_2$, and $\boldsymbol{\nu}''_3$. Both molecular centers of mass are within 1% of the unit cell dimensions of their idealized locations at the origin and cell body center, respectively. In the idealized BCC lattice, each lattice point has eight equidistant nearest neighbors. The rhombohedral distortion accounts for the two neighbors that are somewhat more distant than the closest six. Other minor distortions lead to small differences in the distances to the closest six neighbors.

COPL can be used to verify that the overall transition is consistent with the symmetries of the reference lattice and the daughter structure (Stokes *et al.*, 2007). In addition, COPL provides a complete list of order parameters for the transition. If a single order parameter with the appropriate size and index appears on the list, then it is identified as the primary order parameter. Otherwise, it is identified as a coupled transformation. For the example of MEZDIE01, there is no single primary order parameter consistent with the size (2) and index (48) of the transformation, so the transformation is coupled. The program ISODISPLACE may be used to identify the primary order parameter for coupled transitions (Campbell *et al.*, 2006). Since this identification was not necessary for our purposes, no attempt to further characterize the required coupling was attempted for coupled transformations. COPL output for each of the structures identified with sphere packing reference lattices are summarized in (supplementary) Table 8 available from the journal publisher.

Appendix B
Rod Packing

For 16 of the 70 crystal structures in the data set considered, the center of mass distribution was identified with a rod packing. To illustrate the process of reference lattice assignment, the CSD structure MECKIO is considered in detail below. Details of the assignments for all 16 structures are summarized in (supplementary) Table 6 available from the journal publisher.

CSD structure MECKIO has a monoclinic unit cell with $b/a = 1.6109$, $c/a = 1.1271$, and $\beta = 104.95\,\mathrm{deg}$. The unit parameters can be conveniently represented in matrix form where the matrix columns correspond to the cell vectors and the rows are components of the vectors parallel to orthonormal laboratory frame coordinates,

$$\mathbf{M}_1 = \begin{bmatrix} 1 & 0 & -0.2908 \\ 0 & 1.6109 & 0 \\ 0 & 0 & 1.0889 \end{bmatrix}. \tag{19}$$

The molecular centers of mass are related by a screw axis,

$$\boldsymbol{\nu}_1 = \begin{bmatrix} 0.2050 \\ 1/4 \\ 0.2193 \\ 1 \end{bmatrix} \tag{20}$$

$$\boldsymbol{\nu}_1' = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 2 \end{bmatrix} - \boldsymbol{\nu}_1. \tag{21}$$

Enumeration of the neighboring centers of mass for an arbitrarily chosen reference molecule reveals that there are two equidistant nearest neighbors. Two additional neighbors are within a shell 3% larger than the nearest neighbor distance, but the set of four neighbors are all within a single hemisphere relative to the reference center. Therefore, the set of four neighbors do not indicate a sphere packing.

The nearest neighbors are part of a chain of molecules oriented along the crystallographic a-axis. Therefore, the unit cell is transformed such that the chains are directed along the c-axis, and the other axes are orthogonal. A matrix accomplishing

the desired transformation is

$$\mathbf{T}_{12} = \begin{bmatrix} 0 & 0.2908 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad (22)$$

$$|\mathbf{T}_{12}| = 1. \quad (23)$$

A subsequent rotation about the chain axis orients the chain symmetry elements relative to the a- and b-axes and rescales those axes,

$$\mathbf{T}_{23} = \begin{bmatrix} 0.5814 & 0.5814 & 0 \\ -0.8600 & 0.8600 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (24)$$

$$|\mathbf{T}_{23}| = 1. \quad (25)$$

The product of the transformation matrices gives the overall transformation matrix,

$$\mathbf{T} = \mathbf{T}_{12} \cdot \mathbf{T}_{23}. \quad (26)$$

To determine the fractional coordinates of the centers of mass in the transformed coordinates, it is convenient to define an augmented transformation matrix as follows:

$$\mathbf{S} = \begin{bmatrix} \mathbf{T} & \mathbf{w} \\ \mathbf{0} & \mathbf{1} \end{bmatrix} \quad (27)$$

where w is the origin shift in the original coordinate system,

$$\mathbf{w} = \begin{bmatrix} 0.2050 \\ 1/4 \\ 0.2193 \end{bmatrix}. \quad (28)$$

Transforming the atomic coordinates using S shows that the molecular centers of mass are at Wycoff point a and molecular mirror planes coincide with Wycoff point f of rod group $p\bar{4}2m$. Considering only the x and y coordinates of the rods yields a close approximation to a hexagonal ($p6mm$ planar group) projection. Therefore, MECKIO is characterized as a hexagonal packing of $p\bar{4}2m$ rods.

Appendix C
Other Packings

Twelve of the 70 crystal structures in the data set considered were identified as planar packings, dimer packings, or mixed packings. The procedures for characterizing these structures are similar to those illustrated above for sphere and rod packings. Therefore, details are not given here, but may be found in (supplementary) Table 6 available from the journal publisher.

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Table 1. *Sphere Packings*

Parent	S.G.	W.P.	$\|G\|/Z$	CSD Code(s)
Diamond	Fd3m (no. 227)	a	24	ZNOXAC01
Diam. - Compr.	I41/amd (no. 141)	a	8	FUZLUH, VAFWAA
Diam. - Elong.	I41/a (no. 88)	a	4	KANGUB01
Diam - Ortho.	C2/c (no. 15)	e	2	RASDOE, TFMETH02
BCC	I-43m (no. 217)	a	24	DEQPAQ, HMGETP, HMSIPA HXMTAM07, KELREY, MESIAD MPTHOT01, NIWMIP, POSLOY10 TMEPTC, YEYQAU
	R3c (no. 161)	a	3	TCYMET
	Pbcn (no. 60)	c,d	2/3	YIMWEW
	P-1 (no. 2)	i	1	MEZDIE01, MEZDOK01
	P-1 (no. 2)	i,i,i	1/3	OHABEE
SC	P-43m (no. 215)	a	24	FOHCUA, FUZVOL, JUFWUC
	I-4c2 (no. 120)	c	4	YEMRIR
HCP	P63/m (no. 176)	h	2	CUCZUV
	P-3c1 (no. 165)	d	3	DILWIE01, ZEYHIU
	P-3 (no. 147)	d	3	ZIZHIZ
FCC	P3121 (no. 152)	b	2	MTRETC10
	I-42m (no. 121)	a	8	ZZZKDW01
	I41/acd (no. 142)	a	4	KUJSIR
	P-421c (no. 114)	a	4	ADAMAN08, GERHOA
	Cmce (no. 64)	d,f	1	(MethaneIII)
	C2/c (no. 15)	e	2	REKYUB
	C2/m (no. 12)	i	2	MECKOU
	P21/c (no. 14)	e	1	MECKUA
	P21/c (no. 14)	e	1	TOHSUE
	C2/c (no. 15)	f,f,f,f	1/4	CTBROM, CARBTC07

Table 2. *Rod Packings*

S.G.	Molecule Wyck. Pt.	Rod Symmetry	Latteral Packing	$\|G\|/Z$	CSD Code(s)
P42/nmc (no. 137)	a	p-4m2	8	square	FUZTEZ
Pnma (no. 62)	c	pmcm	2	square	GUTCED, JEYSEL,RIMMOP
C2/c (no. 15)	e	p-4m2	2	hexagonal	BOGMEP
C2/c (no. 15)	e	pmcm	2	hexagonal	MSISUL10, TMGEHS10, TMSNHS10
P21/m (no. 11)	e	p-4m2	2	hexagonal	MECKIO
P21/c (no. 14)	e	pc11	2	hexagonal	QUGBOJ
P21/c (no. 14)	e	p-1	1	hexagonal	DOCNIS
P21/c (no. 14)	e	p-1	1	square	TMSIAD
P21/c (no. 14)	e,e	pmcm	1/2	hexagonal	MXSNOX
P2/c (no. 13)	e,f,g	p-4m2	1/2	hexagonal	RIMNAC
P-1 (no. 2)	i	p-1	1	square	BASXOI
P-1 (no. 2)	i	p-1	1	oblique	XAGXAE

Table 3. *Planar Packings*

S.G.	Molecule Wyck. Pt.	Planar Symmetry	$\|G\|/Z$	CSD Code(s)
P212121 (no. 19)	a	p4mm	1	MZNMOX10
P21/c (no. 14)	e	p2gg	1	CAMPOV, VAVYAS
P21/c (no. 14)	e,e	p6mm	1/2	CANFIG, MXSNOX
P-1 (no. 2)	i,i,i,i	p6mm	1/4	CANFOM

Table 4. *Dimer Packings*

S.G.	Molecule Wyck. Pt.	Dimer Wyck. Pt.	$\|G\|/Z$	CSD Code(s)
Pa-3 (no. 205)	c (3)	a (-3)	3	FOJBUB02, VADRAU
I41/a (no. 88)	f (1)	e (2)*	1	LUFYEQ
P21/c (no. 14)	e (1)	a (-1)	1	CARBTC

Pairs of dimers form quadramers with $S4$ point group symmetry centered at Wyckoff point a.

Table 5. *Mixed Packings*

S.G.	W.P.	$\|G\|/Z$	CSD Code(s)
P-43n (no. 218)	a,c	3	KOXKOX, SENLAY, RUQMEV

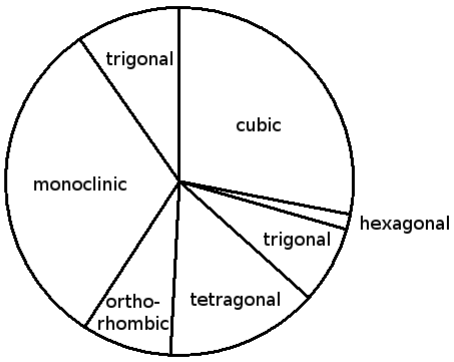

Fig. 1. Crystal systems for crystals of tetrahedral molecules.

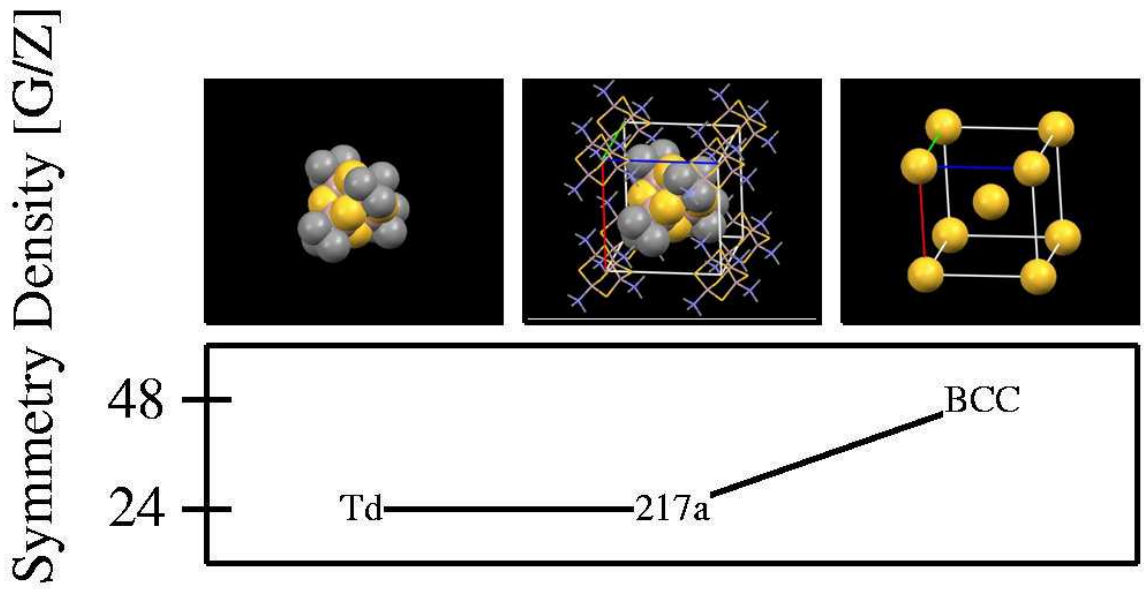

Fig. 2. Symmetry breaking plot for a structure with molecular center of mass lattice coincident with the reference lattice, illustrated using NIWMIP. The figure on the left is an isolated monomer with Td symmetry (G/Z=24/1). The figure on the right is the BCC reference lattice (G/Z=96/2). In the middle is the crystal structure in space group $I\bar{4}3m$ (no. 217) with one molecule at Wyckoff point a emphasized for clarity (G/Z=48/2).

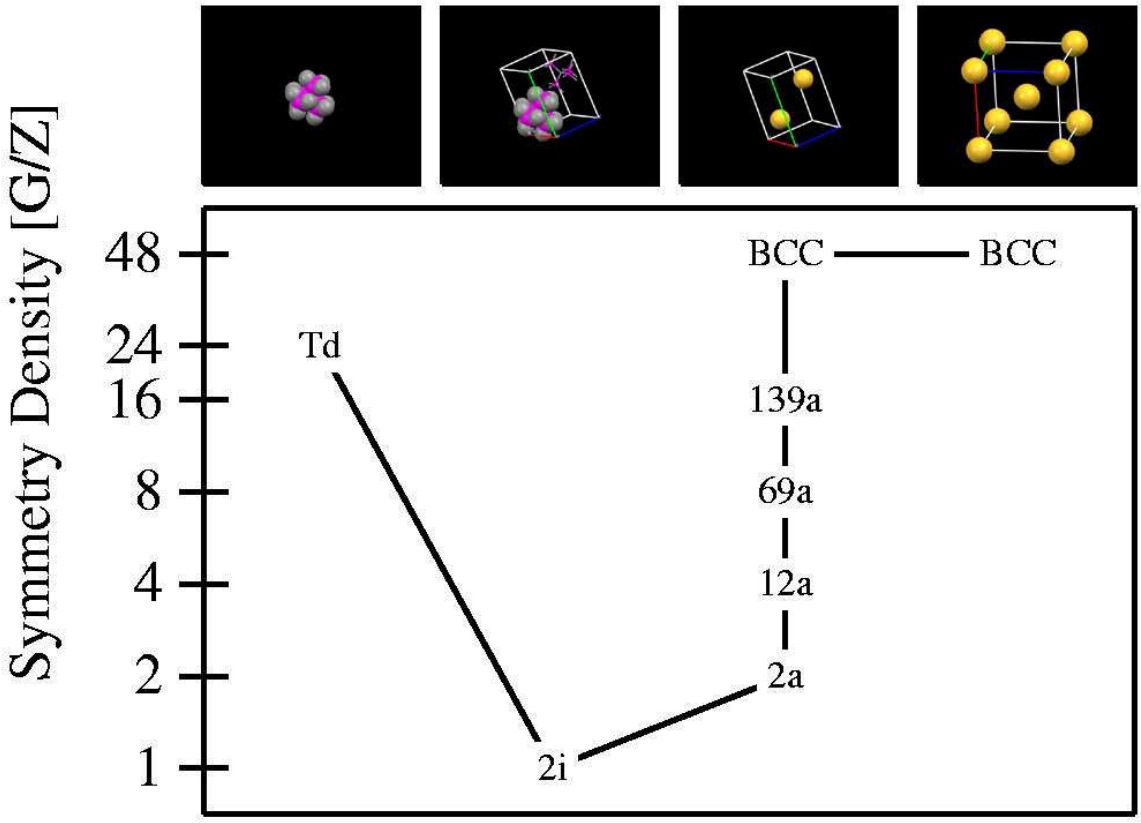

Fig. 3. Symmetry breaking plot for a molecular center of mass lattice not trivially related to the reference lattice, illustrated using MEZDIE01. The figure on the left is an isolated monomer with Td symmetry (G/Z=24/1). The figure on the far right is the BCC reference lattice (G/Z=96/2). Second from the right is the BCC reference lattice in a non-conventional unit cell which may be obtained through a series of perturbations. The illustrated cascade of symmetry-breaking transitions from BCC through tetragonal (139a), orthorhombic (69a), monoclinic (12a), and triclinic (2a) intermediates is not unique. The non-conventional unit cell is similar to the crystal structure with one molecule emphasized for clarity in the second illustration from the left (G/Z=2/2).

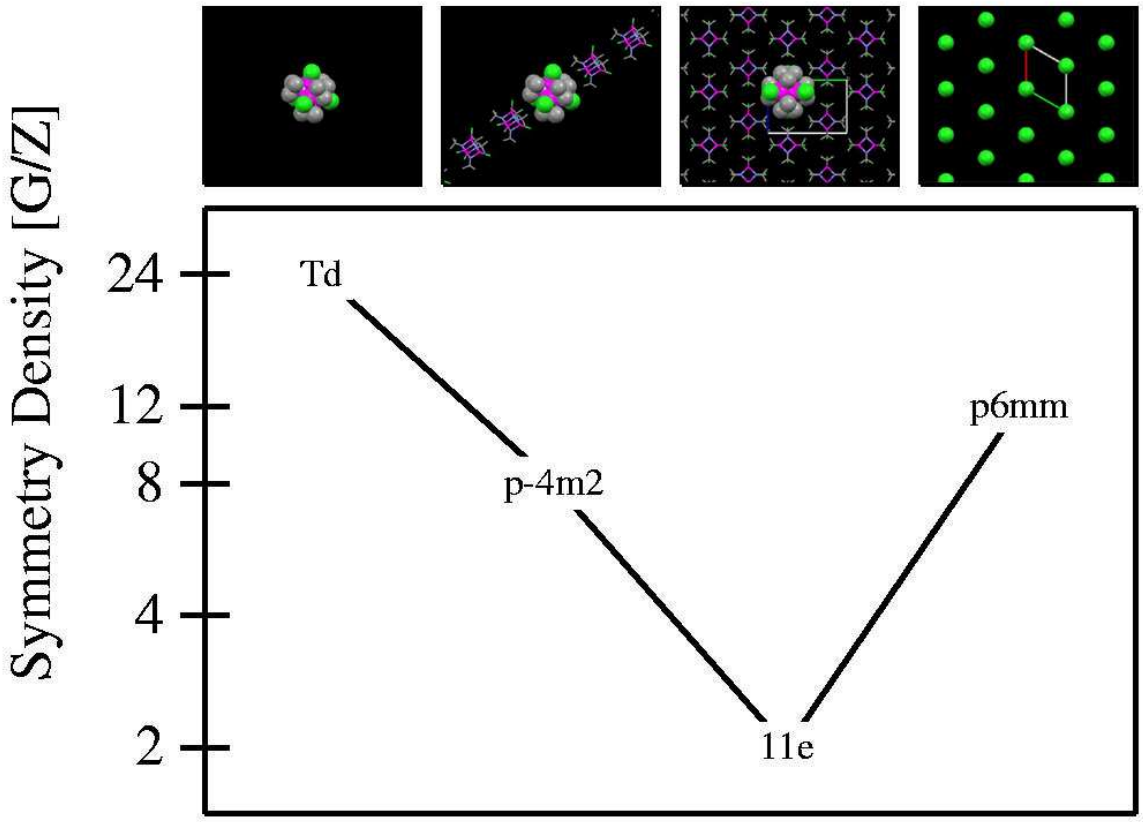

Fig. 4. Symmetry breaking plot for a rod packing, illustrated using MECKIO. The figure on the left is an isolated monomer with Td symmetry (G/Z=24/1). Second from the left is a rod packing with rod group $p\bar{4}m2$ (G/Z=8/1=8). The figure on the far right is a two-dimensional hexagonal packing representing the lateral packing of the rods (G/Z=12/1). Second from the right is the crystal structure with one rod emphasized for clarity (G/Z=4/2). The crystal is viewed end-on to emphasize nearly hexagonal packing of rods.

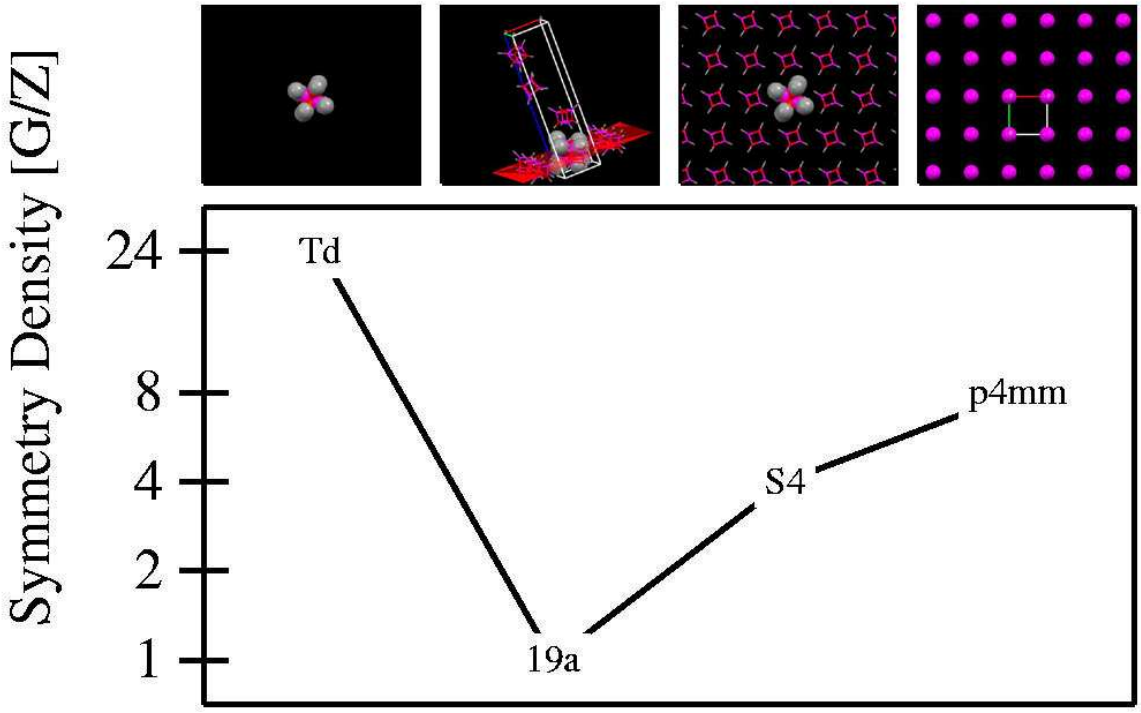

Fig. 5. Symmetry breaking plot for a planar packing, illustrated using MZNMOX10. The figure on the left is an isolated monomer with Td symmetry (G/Z=24/1). On the far right is a two-dimensional square packing representing the center-of-mass lattice in the plane (G/Z=8/1). Second from the right is a planar packing with point group $S4$ (G/Z=4/1). Second from the left is the crystal structure with one plane emphasized for clarity (G/Z=4/4).

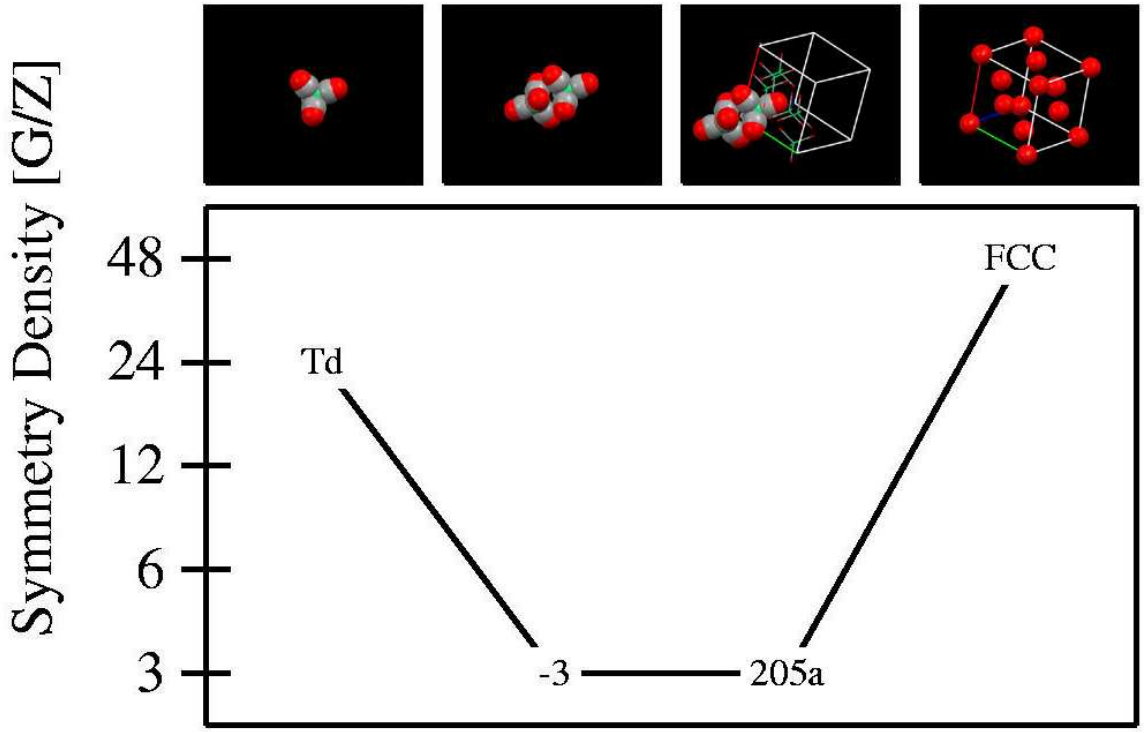

Fig. 6. Symmetry breaking plot for a dimer packing, illustrated using FOJBUB02. The figure on the left is an isolated monomer with Td symmetry (G/Z=24/1). Second from the left is a dimer with $C3i$ point group symmetry (G/Z=6/2). On the far right is the FCC reference lattice (G/Z=192/4). Second from the right is the crystal structure in space group 205 with one dimer at Wyckoff point a emphasized for clarity (G/Z=24/8).

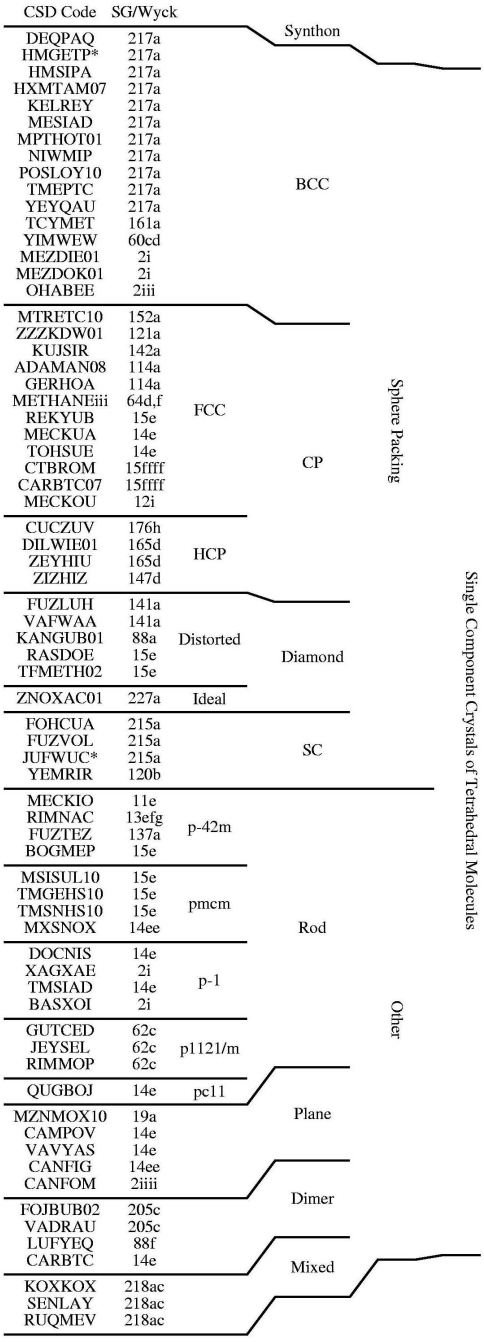

Fig. 7. Tree diagram of the distribution of data set among crystal packing synthons, where spheres and other types of packing form the trunk and the translational arrangements of the structures in our data set form the leaves. Note: Asterisks on JUFWUC and HMGETP are due to space group corrections. See Sec. 2.1 for details.

Synopsis

Experimental crystal structures that are amenable for inclusion in Global Phase Diagrams as previously developed are identified.

Supplementary Material

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.

A

2i P_-1
MEZDIE01

B

a=	9.920097
b=	14.51031
c=	9.135857
alpha=	90.47694
beta=	111.6724
gamma=	89.98776

C

b/a=	1.4627186
c/a=	0.9209443
alpha=	90.47694
beta=	111.67244
gamma=	89.98776

D

6 neighbors within 3% of nearest
next neighbor 11% farther than nearest
sphere packing

E

Matrix Representation

1	0.0003125	-0.340105
0	1.4627185	-0.007593
0	0	0.8558094

a	b	c
1	1.4627186	0.9209443
90.47694	111.67244	89.98776
alpha	beta	gamma

F

i 1

G

Center of Mass Coordinates

x,y,z	0.7605859	0.2506235	0.24179	1
1-x,1-y,1-z	0.2394141	0.7493765	0.75821	1
x=	0.7605859			
y=	0.2506235			
z=	0.24179			

H

Transformation to Reduced Cell

0.5	0.5	0	0.75
0.5	-0.5	0	0.25
0.5	0.5	-1	0.25
0	0	0	1

Det= 0.5

I

Inverse Transformation

1	1	0	-1
1	-1	0	-0.5
1	0	-1	-0.5
0	0	0	1

Det= 2

Matrix Representation

0.330103967	0.329791489	0.340104544
0.727562585	-0.735155941	0.007593356
0.427904687	0.427904687	-0.855809373

a	b	c
0.906321337	0.912315244	0.920944321
107.9992896	107.3143809	107.0838036
alpha	beta	gamma

Normalized Niggli Matrix

1	1.01327063	1.032529194
-0.316067389	-0.302416346	-0.295712962

0,0,0	0.011209412	0.009962353	0.018795882	1	Z'= 1
	-0.011209412	-1.009962353	-1.018795882	1	

	|G|	Z	|G|/Z
Daughter	2	2	1
Ref. Lattice	48	1	48
		2	48
		(size)	(index)

Reduced Cell

Character	44 (aP)	... but close to 5 (cI)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

0.5	-1	-0.5	0
0.5	1	-0.5	-0.5
0.5	0	0.5	-0.5
0	0	0	1

Det= 1

Order Parameter = Coupled

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.

A-D

11e P_21/m
MECKIO

a=	9.5283		
b=	15.3492	b/a=	1.6109065
c=	10.7393	c/a=	1.1270951
alpha=	90	alpha=	90
beta=	104.954	beta=	104.954
gamma=	90	gamma=	90

2 nearest neighbors
2 next neighbors not coplanar

Hexagonal packing of p-42m rods

E

Matrix Representation

1	0	-0.29084
0	1.6109065	0
0	0	1.0889241

a	b	c
1	1.6109065	1.1270951
90	104.954	90
alpha	beta	gamma

H

Transformation to Rod Coordinates

0	0.29084	1	0.20498
1	0	0	0.25
0	1	0	0.219284
0	0	0	1

Det= 1

I

Inverse Transformation

0	1	0	-0.25
0	0	1	-0.219284
1	0	-0.29084	-0.141203
0	0	0	1

Det= 1

F

Center of Mass Coordinates

	e m				
i	x,1/4,z	0.2049796	0.25	0.2192841	1
	1-x,3/4,1-z	0.7950204	0.75	0.7807159	1
	x=	0.2049796			
	z=	0.2192841			

J

rod axis:

1	0	0

rod origin:

0.20498	0.25	0.219284

Transformation to orthogonal axes:
0.29084

G

Molecular 3-fold axes

	f 1				
i	x,y,z	0.0917	0.1478	0.2244	1
i	x,1/2-y,z	0.0917	0.3522	0.2244	1
	e m				
i	x,1/4,z	0.2782	0.25	0.0701	1
i		0.3715	0.25	0.3735	1

Rotation about rod and rescaling:

0.581364682	0.581364682	0	0
-0.860045365	0.860045365	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.860045365	-0.581364682	0	0
0.860045365	0.581364682	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

45 degrees

Rescaling parameter:

0.822173817

Matrix Representation

0	0	1
0.93652412	0.93652412	0
-0.93652412	0.93652412	0

a	b	c
1.324445112	1.324445112	1
89.99999743	90.00000257	90
alpha	beta	gamma

p-42m (#37)
2nd setting

a m2m

0,0,0	0	0	0	1
	0.103626103	0.756419262	0.426754	1

f m

-x,-x,z	-0.09087082	-0.084922453	-0.114767	1
x,x,z	0.084922453	0.09087082	-0.114767	1
x,-x,-z	0.086730387	-0.086730387	0.116609	1
-x,x,-z	-0.089655658	0.089655658	0.121668	1
error	-0.003122377	0.002825991	0.002186	

x= 0.088044829
z= -0.116953091

		|G|	Z	|G|/Z
Daughter	11e	4	2	2
Rod	37a	8	1	8
			2	4
			(size)	(index)

Z'= 1

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.

A-E

14e P_21/c
CAMPOV

a=	10.3894		
b=	14.6835	b/a=	1.4133155
c=	16.9885	c/a=	1.6351762
alpha=	90	alpha=	90
beta=	91.61	beta=	91.61
gamma=	90	gamma=	90

3 neighbors within 4% of nearest
next neighbor 26% farther than nearest

planar packing

Matrix Representation

1	0	-0.045942
0	1.4133155	0
0	0	1.6345307

a	b	c
1	1.4133155	1.6351762
90	91.61	90
alpha	beta	gamma

Transformation to Planar Coordinates

0	0.045942	1	0
1	0	0	0
0	1	0	0
0	0	0	1

Det= 1

G

Inverse Transformation

0	1	0	0
0	0	1	0
1	0	-0.045942	0
0	0	0	1

Det= 1

Center of Mass Coordinates

e 1

x,y,z	0.1712083	0.0255667	0.2124792	1
1-x,1/2+y,1	0.8287917	0.5255667	0.2875208	1
1-x,1-y,1-z	0.8287917	0.9744333	0.7875208	1
x,1/2-y,1/2+	0.1712083	0.4744333	0.7124792	1

F

x= 0.1712083
y= 0.0255667
z= 0.2124792

plane normal:

1	0	0

plane origin:

0	0	0

Transformation to orthogonal axes:
0.045942

H

Rotation about plane normal and rescaling:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

0 degrees

I

Matrix Representation

8.65761E-17	0	1
1.413315495	1.02981E-16	0
0	1.634530713	0

a	b	c
1.413315495	1.634530713	1
90	90	90
alpha	beta	gamma

p2gg (#8) in projection

$2_1/c$ when accounting for 3rd dimension

J

x,y,z	0.025566667	0.212479167	0.161447	1
1/2+x,1/2-y,-z	0.525566667	0.287520833	0.815582	1
-x,-y,-z	0.974433333	0.787520833	0.792611	1
1/2-x,1/2+y,z	0.474433333	0.712479167	0.138476	1
x=	0.025566667			
y=	0.212479167			
z=	0.161446598			
error=	0	0	0	

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Plane	$2_1/c$	4	4	1
			1 (size)	1 (index)

Z'= 4

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+.

A-E

14e P_21/c
CARBTC

a=	9.07912		
b=	5.7643	b/a=	0.6348963
c=	9.2014	c/a=	1.0134683
alpha=	90	alpha=	90
beta=	104.295	beta=	104.295
gamma=	90	gamma=	90

1 nearest neighbor
3 neighbors within 6% of nearest
next neighbor 11% farther than nearest

Matrix Representation

1	0	-0.25024
0	0.6348963	0
0	0	0.9820885

a	b	c
1	0.6348963	1.0134683
90	104.295	90
alpha	beta	gamma

G

Transformation to Reduced Cell

0	-1	0	1
-1	0	0	1
0	0	-1	1
0	0	0	1

Det= 1

Inverse Transformation

0	-1	0	1
-1	0	0	1
0	0	-1	1
0	0	0	1

Det= 1

F

Center of Mass Coordinates

e 1

i	x,y,z	0.248	0.067	0.157	1
ii	1-x,1/2+y,1	0.752	0.567	0.343	1
i	1-x,1-y,1-z	0.752	0.933	0.843	1
ii	x,1/2-y,1/2+	0.248	0.433	0.657	1
	x=	0.248			
	y=	0.067			
	z=	0.157			

H

Matrix Representation

0	-1	0.250239959
-0.634896334	0	0
0	0	-0.982088534

a	b	c
0.634896334	1	1.013468266
104.295	90	90
alpha	beta	gamma

I

Normalized Niggli Matrix

1	2.480814901	2.548089455
-0.620799018	9.77836E-17	9.64841E-17

J

Reduced Cell

Character	35 (mP)	... but close to 23 (oC)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

K

0.933	0.752	0.843	1	Z'= 4
0.433	0.248	0.657	1	
0.067	0.248	0.157	1	
0.567	0.752	0.343	1	

dimers:

Dimer Coordinates (a), -1 WP symmetry ensures Cs dimer symmetry
4 nearest neighbors, all coplanar (bc-plane)
next neighbor 6% farther, also co-planar
next neighbor 67% farther than nearest
packing of dimers

Transformation to Reduced Cell

0	0	-1	0
-0.5	0.5	0	0
0.5	0.5	0	0
0	0	0	1

Det= 0.5

Inverse Transformation

0	-1	1	0
0	1	1	0
-1	0	0	0
0	0	0	1

Det= 2

Dimer Center of Mass Coordinates

	a -1				
i	0,0,0	0	0	0	1
ii	0,1/2,1/2	0	0.5	0.5	1

O

Matrix Representation

-0.125119979	-0.125119979	-1
-0.317448167	0.317448167	0
0.491044267	0.491044267	0

a	b	c
0.597957206	0.597957206	1
77.92184748	77.92184748	64.13091485
alpha	beta	gamma

S

		|G|	Z	|G|/Z
Daughter	14e	4	4	1
Cs Dimers	12a	4	1	4
Ref. Lattice	166a	12	1	12
			1 (size)	3 (index)

P

Normalized Niggli Matrix

1	1	2.796789577
0.349934254	0.349934254	0.436316354

Q

Reduced Cell

Character	10 (mC)	... but close to 9 (hR)	
Type	I		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	N/A	|a.b|≤a.a/2	True

R

0,0,0	0	0	0	1	Z' = 1
	0	1	0	1	

Transformation to Conventional Cell

1	-1	-1	0
0	1	-1	0
0	0	3	0
0	0	0	1

Det= 3

Overall Transformation

-0.666667	0	2	0
-0.333333	1	1	0
-0.333333	0	0	0
0	0	0	1

Det= 0.666667

Order Parameter = F2+

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-).

A-E

218a,c P_-4_3_n
KOXKOX
SENLAY

b/a=	1
c/a=	1
alpha=	90
beta=	90
gamma=	90

Matrix Representation

1	0	0
0	1	0
0	0	1

a	b	c
1	1	1
90	90	90
alpha	beta	gamma

G

Transformation to Reduced Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

F

12 nearest neighbors
next neighbor 55% farther

2 nearest neighbors
next neighbor 12% farther

Center of Mass Coordinates

a -43m	Origin Choice 2			
0,0,0	0	0	0	1
1/2,1/2,1/2	0.5	0.5	0.5	1
c -4..	Origin Choice 2			
1/4,1/2,0	0.25	0.5	0	1
3/4,1/2,0	0.75	0.5	0	1
0,1/4,1/2	0	0.25	0.5	1
0,3/4,1/2	0	0.75	0.5	1
1/2,0,1/4	0.5	0	0.25	1
1/2,0,3/4	0.5	0	0.75	1

Matrix Representation

1	0	0
0	1	0
0	0	1

a	b	c
1	1	1
90	90	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
0	0	0

	|G|	Z	|G|/Z
Daughter	218a,c	24	8	3
Ref. Lattice	223a,c	48	8	6
			1 (size)	2 (index)

Reduced Cell

Character	3 (cP)		
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

0,0,0	0	0	0	1	Z' = 2
1/2,1/2,1/2	0.5	0.5	0.5	1	
1/4,1/2,0	0.25	0.5	0	1	Z' = 6
3/4,1/2,0	0.75	0.5	0	1	
0,1/4,1/2	0	0.25	0.5	1	
0,3/4,1/2	0	0.75	0.5	1	
1/2,0,1/4	0.5	0	0.25	1	
1/2,0,3/4	0.5	0	0.75	1	

Transformation to Conventional Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Order Parameter = GM2-

Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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

Table 6: Structure Classification

Cubic (Isometric) Crystal Structures (195-230)

227a F_d_3_m

1 ZNOXAC01

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

4 equidistant neighbors
next neighbor 63% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Transformation to Reduced Cell

0	0.5	0.5	0
0.5	0	0.5	0
0.5	0.5	0	0
0	0	0	1

Det= 0.25

Inverse Transformation

-1	1	1	0
1	-1	1	0
1	1	-1	0
0	0	0	1

Det= 4

Matrix Representation

0	0.5	0.5
0.5	0	0.5
0.5	0.5	0

a b c
0.707106781 0.707106781 0.707106781

Reduced Cell

60	60	60	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	1
0.5	0.5	0.5

Daughter 227a
Ref. Lattice Diamond

|G|	Z	|G|/Z	
48	2	24	
48	2	24	
	1	1	
	(size)	(index)	

Character 1 (cF)
Type I
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B N/A
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 True
|a.b|≤|a.a/2 True

Transformation to Conventional Cell

-1	1	1	0
1	-1	1	0
1	1	-1	0
0	0	0	1

Det= 4

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates

a -43m Origin Choice 2

1/8,1/8,1/8	0.125	0.125	0.125	1
7/8,3/8,3/8	0.875	0.375	0.375	1
1/8,5/8,5/8	0.125	0.625	0.625	1
7/8,7/8,7/8	0.875	0.875	0.875	1
5/8,1/8,5/8	0.625	0.125	0.625	1
3/8,3/8,7/8	0.375	0.375	0.875	1
5/8,5/8,1/8	0.625	0.625	0.125	1
3/8,7/8,3/8	0.375	0.875	0.375	1

1/8,1/8,1/8 0.125 0.125 0.125 1
7/8,7/8,7/8 -0.125 0.875 0.875 1
1.125 0.125 0.125 1
0.875 0.875 0.875 1
0.125 1.125 0.125 1
0.875 0.875 -0.125 1
0.125 0.125 1.125 1
0.875 -0.125 0.875 1

Z' = 2

Order Parameter = GM1+

217a I_-4_3_m

2 DEQPAQ
3 HMGETP *
4 HMSIPA
5 HXMTAM07
6 KELREY
7 MESIAD
8 MPTHOT01
9 NIWMIP
10 POSLOY10
11 TMEPTC
12 YEYQAU

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

* Very slightly distorted molecules or mislabeled as 197a by authors

8 nearest neighbors
next neighbor 15% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
90 90 90

Transformation to Reduced Cell

-0.5	0.5	0.5	0
0.5	-0.5	0.5	0
0.5	0.5	-0.5	0
0	0	0	1

Det= 0.5

Inverse Transformation

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Matrix Representation

-0.5	0.5	0.5
0.5	-0.5	0.5
0.5	0.5	-0.5

a b c
0.866025404 0.866025404 0.866025404
109.4712206 109.4712206 109.4712206

Reduced Cell

alpha	beta	gamma	
109.4712206	109.4712206	109.4712206	

Normalized Niggli Matrix

1	1	1
-0.333333333	-0.333333333	-0.333333333

Daughter 217a
Ref. Lattice BCC

|G|	Z	|G|/Z	
24	1	24	
48	1	48	
	1	2	
	(size)	(index)	

Character 5 (cI)
Type II
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B Equal
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 True
|a.b|≤|a.a/2 True

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates

a -43m Origin Choice 2

0,0,0 0 0 0 1
1/2,1/2,1/2 0.5 0.5 0.5 1

0,0,0 0 0 0 1
1 1 1 1

Z' = 1

Order Parameter = GM2-

215a P_-4_3_m

13 FOHCUA
14 FUZVOL
15 JUFWUC *

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

* Very slightly distorted molecules or mislabeled as 195a by authors

6 nearest neighbors
next neighbor 41% farther
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Transformation to Reduced Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Reduced Cell

alpha	beta	gamma	
90	90	90	

Normalized Niggli Matrix

1	1	1
0	0	0

Daughter 215a
Ref. Lattice SC

|G|	Z	|G|/Z	
24	1	24	
48	1	48	
	1	2	
	(size)	(index)	

Character 3 (cP)
Type II
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B True
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 True
|a.b|≤|a.a/2 True

Transformation to Conventional Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates

a -43m Origin Choice 2

0,0,0 0 0 0 1

0,0,0 0 0 0 1

Z' = 1

Order Parameter = GM2-

218a,c P_-4_3_n

16 KOXKOX
17 SENLAY

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Transformation to Reduced Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Reduced Cell

alpha	beta	gamma	
90	90	90	

Normalized Niggli Matrix

1	1	1
0	0	0

Daughter 218a,c
Ref. Lattice 223a,c

|G|	Z	|G|/Z	
24	8	3	
48	8	6	
	1	2	
	(size)	(index)	

Character 3 (cP)
Type II
b.bza.a True
c.czb.b True
2|D+E+F| ≤ A+B True
|b.c|≤|b.b/2 True
|a.c|≤|a.a/2 True
|a.b|≤|a.a/2 True

Transformation to Conventional Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates

a 12 nearest neighbors
next neighbor 55% farther

a -43m Origin Choice 2

0,0,0 0 0 0 1
1/2,1/2,1/2 0.5 0.5 0.5 1

c -4.. Origin Choice 2

c 2 nearest neighbors
next neighbor 12% farther

1/4,1/2,0 0.25 0.5 0 1
3/4,1/2,0 0.75 0.5 0 1
0,1/4,1/2 0 0.25 0.5 1
0,3/4,1/2 0 0.75 0.5 1
1/2,0,1/4 0.5 0 0.25 1
1/2,0,3/4 0.5 0 0.75 1

0,0,0 0 0 0 1
1/2,1/2,1/2 0.5 0.5 0.5 1

1/4,1/2,0 0.25 0.5 0 1
3/4,1/2,0 0.75 0.5 0 1
0,1/4,1/2 0 0.25 0.5 1
0,3/4,1/2 0 0.75 0.5 1
1/2,0,1/4 0.5 0 0.25 1
1/2,0,3/4 0.5 0 0.75 1

Z' = 2

Z' = 6

Order Parameter = GM2-

218a,d P_-4_3_n

18 RUQMEV

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Transformation to Reduced Cell

1	0	0	-0.5
0	1	0	-0.5
0	0	1	-0.5
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0.5
0	1	0	0.5
0	0	1	0.5
0	0	0	1

Det= 1

Matrix Representation

1	0	0
0	1	0
0	0	1

a b c
1 1 1
90 90 90

Reduced Cell

alpha	beta	gamma	
90	90	90	

Normalized Niggli Matrix

1	1	1
0	0	0

See #16 and #17 above.

Center of Mass Coordinates

a 12 nearest neighbors
next neighbor 55% farther
distorted icosahedral coordination

a -43m Origin Choice 2

0,0,0 0 0 0 1
1/2,1/2,1/2 0.5 0.5 0.5 1

d -4.. Origin Choice 2

d 2 nearest neighbors
next neighbor 12% farther
pairs of rods in 3 orthogonal directions

1/4,0,1/2 0.25 0 0.5 1
3/4,0,1/2 0.75 0 0.5 1
1/2,1/4,0 0.5 0.25 0 1
1/2,3/4,0 0.5 0.75 0 1

c -4..

1/2,1/2,1/2 0.5 0.5 0.5 1
0,0,0 1 1 1 1
3/4,1/2,0 0.75 0.5 1 1
1/4,1/2,0 1.25 0.5 1 1
0,3/4,1/2 1 0.75 0.5 1
0,1/4,1/2 1 1.25 0.5 1

See above. 0,1/2,1/4 0 0.5 0.25 1 1/2,0,3/4 0.5 1 0.75 1
0,1/2,3/4 0 0.5 0.75 1 1/2,0,1/4 0.5 1 1.25 1

205c P_a_-3
19 FOJBUB02

Matrix Representation
1 0 0
0 1 0
0 0 1
a b c
1 1 1
90 90 90
alpha beta gamma

Transformation to Reduced Cell
1 0 0 0
0 1 0 0
0 0 1 0
0 0 0 1
Det= 1

Inverse Transformation
1 0 0 0
0 1 0 0
0 0 1 0
0 0 0 1
Det= 1

Matrix Representation
1 0 0
0 1 0
0 0 1
a b c
1 1 1
90 90 90
alpha beta gamma

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

1 nearest neighbor
next neighbor 33% farther
dimer packing

Center of Mass Coordinates
c .3. Origin Choice 2

i	x,x,x	0.1220303	0.1220303	0.1220303	1	x,x,x	0.1220303	0.1220303	0.1220303	1	Z' = 8
ii	1/2-x,1-x,1	0.3779697	0.8779697	0.6220303	1		0.3779697	0.8779697	0.6220303	1	
iii	1-x,1/2+x,1	0.8779697	0.6220303	0.3779697	1		0.8779697	0.6220303	0.3779697	1	
iv	1/2+x,1/2-x	0.6220303	0.3779697	0.8779697	1		0.6220303	0.3779697	0.8779697	1	
i	1-x,1-x,1-x	0.8779697	0.8779697	0.8779697	1		0.8779697	0.8779697	0.8779697	1	
ii	1/2+x,x,1/2	0.6220303	0.1220303	0.3779697	1		0.6220303	0.1220303	0.3779697	1	
iii	x,1/2-x,1/2-	0.1220303	0.3779697	0.6220303	1		0.1220303	0.3779697	0.6220303	1	
iv	1/2-x,1/2+x	0.3779697	0.6220303	0.1220303	1		0.3779697	0.6220303	0.1220303	1	
	x=	0.1220303				x=	0.1220303				

dimers:

Transformation to Reduced Cell
0 0.5 0.5 0
0.5 0 0.5 0
0.5 0.5 0 0
0 0 0 1
Det= 0.25

Matrix Representation
0 0.5 0.5
0.5 0 0.5
0.5 0.5 0
a b c
0.707106781 0.707106781 0.707106781
60 60 60
alpha beta gamma

Inverse Transformation
-1 1 1 0
1 -1 1 0
1 1 -1 0
0 0 0 1
Det= 4

Normalized Niggli Matrix
1 1 1
0.5 0.5 0.5

Dimer Coordinates (a), -3 WP symmetry ensures C3i dimer symmetry
12 nearest neighbors
next neighbor 41% farther
sphere packing (of dimers)

Dimer Center of Mass Coordinates
a .-3. Origin Choice 2

i	0,0,0	0	0	0	1	0,0,0	0	0	0	1	Z' = 1
ii	1/2,0,1/2	0.5	1	0.5	1		1	0	1	1	
iii	0,1/2,1/2	1	0.5	0.5	1		0	1	1	1	
iv	1/2,1/2,0	0.5	0.5	1	1		1	1	0	1	

Reduced Cell
Character 1 (cF)
Type I
b.b≥a.a True |b.c|≤b.b/2 True
c.c≥b.b True |a.c|≤a.a/2 True
2|D+E+F| ≤ A+B N/A |a.b|≤a.a/2 True

	|G|	Z	|G|/Z
Daughter	205c	24	8	3
C3i Dimers	205a	24	4	6
Ref. Lattice	FCC	48	1	48
			4	8
			(size)	(index)

Transformation to Conventional Cell
-1 1 1 0
1 -1 1 0
1 1 -1 0
0 0 0 1
Det= 4

Overall Transformation
1 0 0 0
0 1 0 0
0 0 1 0
0 0 0 1
Det= 1

Order Parameter = X5+

205c P_a_-3
20 VADRAU

Matrix Representation
1 0 0
0 1 0
0 0 1
a b c
1 1 1
90 90 90
alpha beta gamma

Transformation to Reduced Cell
1 0 0 0.5
0 1 0 0.5
0 0 1 0.5
0 0 0 1
Det= 1

Inverse Transformation
1 0 0 -0.5
0 1 0 -0.5
0 0 1 -0.5
0 0 0 1
Det= 1

Matrix Representation
1 0 0
0 1 0
0 0 1
a b c
1 1 1
90 90 90
alpha beta gamma

Normalized Niggli Matrix
1 1 1
0 0 0

b/a= 1
c/a= 1
alpha= 90
beta= 90
gamma= 90

1 nearest neighbor
next neighbor 25% farther
dimer packing

See #19 above.

See above.

Center of Mass Coordinates
c .3. Origin Choice 2

i	x,x,x	0.371591	0.371591	0.371591	1		-0.128409	-0.128409	-0.128409	1	
ii	1/2-x,1-x,1	0.128409	0.628409	0.871591	1		-0.371591	0.128409	0.371591	1	
iii	1-x,1/2+x,1	0.628409	0.871591	0.128409	1		0.128409	0.371591	-0.371591	1	
iv	1/2+x,1/2-x	0.871591	0.128409	0.628409	1		0.371591	-0.371591	0.128409	1	
i	1-x,1-x,1-x	0.628409	0.628409	0.628409	1	x,x,x	0.128409	0.128409	0.128409	1	
ii	1/2+x,x,1/2	0.871591	0.371591	0.128409	1		0.371591	-0.128409	-0.371591	1	
iii	x,1/2-x,1/2-	0.371591	0.128409	0.871591	1		-0.128409	-0.371591	0.371591	1	
iv	1/2-x,1/2+x	0.128409	0.871591	0.371591	1		-0.371591	0.371591	-0.128409	1	
	x=	0.371591				x=	0.128409				

Hexagonal Crystal Structures (168-194)

176h P_63/m
21 CUCZUV

Matrix Representation
1 -0.5 0
0 0.8660254 0
0 0 0.8899173
a b c
1 1 0.8899173
90 90 120
alpha beta gamma

Transformation to Reduced Cell
0.666667 -0.333333 0 0
0.333333 0.333333 0 0
0 0 1 0.5
0 0 0 1
Det= 0.333333

Inverse Transformation
1 1 0 0
-1 2 0 0
0 0 1 -0.5
0 0 0 1
Det= 3

Matrix Representation
0.5 -0.5 0
0.288675135 0.288675135 0
0 0 0.889917318
a b c
0.577350269 0.577350269 0.889917318
90 90 120
alpha beta gamma

Normalized Niggli Matrix
1 1 2.375858497
0 0 -0.5

a= 15.7954
b= 15.7954 b/a= 1
c= 14.0566 c/a= 0.8899173
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 120 gamma= 120

12 neighbors within 15% of nearest
next neighbor 49% farther than nearest
sphere packing

Center of Mass Coordinates
h m..

	x,y,1/4	0.3612963	0.3339991	0.25	1	2/3,1/3,3/4	0.695295357	0.306701964	-0.25	1	Z'= 2
	1-y,x-y,1/4	0.6660009	0.0272971	0.25	1		0.693298036	-0.611406607	-0.25	1	
	y-x,1-x,1/4	-0.027297	0.6387038	0.25	1		0.611406607	1.304704643	-0.25	1	
	1-x,1-y,3/4	0.6387038	0.6660009	0.75	1		1.304704643	0.693298036	0.25	1	
	y,y-x,3/4	0.3339991	-0.027297	0.75	1		0.306701964	-0.388593393	0.25	1	cr/ar= 1.54
	x-y,x,3/4	0.0272971	0.3612963	0.75	1	1/3,2/3,1/4	0.388593393	0.695295357	0.25	1	cr/ar_ideal= 1.63
	x=	0.3612963									slightly compressed vs. ideal HCP
	y=	0.3339991				error	0.05526006	0.02862869	0		

Reduced Cell
Character 12 (hP)
Type II
b.b≥a.a True |b.c|≤b.b/2 True
c.c≥b.b True |a.c|≤a.a/2 True
2|D+E+F| ≤ A+B True |a.b|≤a.a/2 True

	|G|	Z	|G|/Z
Daughter	176h	12	6	2
Ref. Lattice	HCP	24	2	12
			3	6
			(size)	(index)

Transformation to Conventional Cell
1 0 0 0
0 1 0 0
0 0 1 0
0 0 0 1
Det= 1

Overall Transformation
1 1 0 0
-1 2 0 0
0 0 1 -0.5
0 0 0 1
Det= 3

Order Parameter = K4

Trigonal Crystal Structures (143-167)

165d P_-3_c_1
22 DILWIE01

Matrix Representation
1 -0.5 0
0 0.8660254 0
0 0 3.072783
a b c

Transformation to Reduced Cell
1 0 0 0
0 1 0 0
0 0 0.5 0
0 0 0 1
Det= 0.5

Matrix Representation
1 -0.5 0
0 0.866025404 0
0 0 1.536391496
a b c

a= 10.442
b= 10.442 b/a= 1
c= 32.086 c/a= 3.072783
alpha= 90 alpha= 90

	|G|	Z	|G|/Z
Daughter	165d	12	4	3
Ref. Lattice	HCP	24	2	12
			2	4
			(size)	(index)

Transformation to Conventional Cell
1 0 0 0
0 1 0 0
0 0 1 0
0 0 0 1
Det= 1

beta= 90 beta= 90 1 1 3.072783
gamma= 120 gamma= 120 90 90 120
alpha beta gamma

12 neighbors within 6% of nearest
next neighbor 46% farther than nearest
sphere packing

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	2	0
0	0	0	1

Det= 2

Center of Mass Coordinates
d 3..

1/3,2/3,z	0.3333333	0.6666667	0.1216413	1
2/3,1/3,1/2	0.6666667	0.3333333	0.3783587	1
2/3,1/3,1-z	0.6666667	0.3333333	0.8783587	1
1/3,2/3,1/2	0.3333333	0.6666667	0.6216413	1

z= 0.1216413

1 1 1.536391496
90 90 120
alpha beta gamma

Normalized Niggli Matrix

1	1	2.360498829
0	0	-0.5

2|D+E+F| ≤ A+B: True

Reduced Cell

Character	12 (hP)		
Type	II		
b.b≥a.a	True	|b.c|≤|b.b/2	True
c.c≥b.b	True	|a.c|≤|a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤|a.a/2	True

Overall Transformation

1	0	0	0
0	1	0	0
0	0	2	0
0	0	0	1

Det= 2

1/3,2/3,1/4	0.333333333	0.666666667	0.243282667	1
2/3,1/3,3/4	0.666666667	0.333333333	0.756717333	1
	0.666666667	0.333333333	1.756717333	1
	0.333333333	0.666666667	1.243282667	1

Z'= 2

Order Parameter = A2

cr/ar= 1.54
error 0 0 -0.006717333 cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

165d P_-3_c_1
23 ZEYHIU
a= 10.7713
b= 10.7713 b/a= 1
c= 32.7927 c/a= 3.0444515
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 120 gamma= 120

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	3.0444515	

a b c
1 1 3.0444515

Transformation to Reduced Cell

-1	0	0	1
0	-1	0	1
0	0	0.5	0
0	0	0	1

Det= 0.5

Inverse Transformation

-1	0	0	1
0	-1	0	1
0	0	2	0
0	0	0	1

Det= 2

Matrix Representation

-1	0.5	0
0	-0.866025404	0
0	0	1.522225729

a b c
1 1 1.522225729

90 90 120
alpha beta gamma

Normalized Niggli Matrix

1	1	2.317171172
0	0	-0.5

See #22 above.

12 neighbors within 10% of nearest
next neighbor 48% farther than nearest
sphere packing

See above.

Center of Mass Coordinates
d 3..

1/3,2/3,z	0.3333333	0.6666667	0.3835717	1
2/3,1/3,1/2	0.6666667	0.3333333	0.1164283	1
2/3,1/3,1-z	0.6666667	0.3333333	0.6164283	1
1/3,2/3,1/2	0.3333333	0.6666667	0.8835717	1

z= 0.3835717

2/3,1/3,3/4	0.666666667	0.333333333	0.767143316	1
1/3,2/3,1/4	0.333333333	0.666666667	0.232856684	1
	0.333333333	0.666666667	1.232856684	1
	0.666666667	0.333333333	1.767143316	1

Z'= 2

cr/ar= 1.52
error 0 0 -0.017143316 cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

161a R_3_c
24 TCYMET
a= 9.0622
b= 9.0622 b/a= 1
c= 11.6253 c/a= 1.2828342
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 120.00 gamma= 120

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	1.2828342	

a b c
1 1 1.2828342

Transformation to Reduced Cell

0.333333	-0.666667	0.333333	0
0.666667	-0.333333	-0.333333	0
0.166667	0.166667	0.166667	0
0	0	0	1

Det= 0.166667

Inverse Transformation

0	1	2	0
-1	0	2	0
1	-1	2	0
0	0	0	1

Det= 6

Matrix Representation

0	-0.5	0.5
0.577350269	-0.288675135	-0.288675135
0.213805698	0.213805698	0.213805698

a b c
0.615667288 0.615667288 0.615667288
108.6085285 108.6085285 108.6085285

90 90 120
alpha beta gamma

Normalized Niggli Matrix

1	1	1
-0.319100381	-0.319100381	-0.319100381

Daughter	161a	6	2	3
Ref. Lattice	BCC	48	1	48
			2	16
			(size)	(index)

Reduced Cell

Character	4 (hR)	… but very close to 5 (cI)	
Type	II		
b.b≥a.a	True	|b.c|≤|b.b/2	True
c.c≥b.b	True	|a.c|≤|a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤|a.a/2	True

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

0	-1	1	0
1	0	1	0
-1	1	1	0
0	0	0	1

Det= 3

8 neighbors within 5% of nearest
next neighbor 17% farther than nearest
sphere packing

Center of Mass Coordinates
a 3.

0,0,z	0	0	0.0004	1
0,0,1/2+z	0	0	0.5004	1
2/3,1/3,1/3	0.6666667	0.3333333	0.3337	1
2/3,1/3,5/6	0.6666667	0.3333333	0.8337	1
1/3,2/3,2/3	0.3333333	0.6666667	0.6671	1
1/3,2/3,1/6	0.3333333	0.6666667	0.1671	1

z= 0.0004

0,0,0	0.0008	0.0008	0.0008	1
	1.0008	1.0008	1.0008	1
	1.0008	0.0008	1.0008	1
	2.0008	1.0008	2.0008	1
	2.0008	1.0008	1.0008	1
	1.0008	0.0008	0.0008	1

Z'= 1

Order Parameter = Coupled

error 0.0008 0.0008 0.0008

147d P_-3
25 ZIZHIZ
a= 9.168711
b= 9.168711 b/a= 1
c= 13.88732 c/a= 1.514642
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 120 gamma= 120

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	1.514642	

a b c
1 1 1.514642

Transformation to Reduced Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

1	-0.5	0
0	0.866025404	0
0	0	1.514642025

a b c
1 1 1.514642025

90 90 120
alpha beta gamma

Normalized Niggli Matrix

1	1	2.294140465
0	0	-0.5

Daughter	147d	6	2	3
Ref. Lattice	HCP	24	2	12
			1	4
			(size)	(index)

Reduced Cell

Character	12 (hP)		
Type	II		
b.b≥a.a	True	|b.c|≤|b.b/2	True
c.c≥b.b	True	|a.c|≤|a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤|a.a/2	True

Transformation to Conventional Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

12 neighbors within 6% of nearest
next neighbor 45% farther than nearest
sphere packing

Center of Mass Coordinates
d 3..

1/3,2/3,z	0.3333333	0.6666667	0.2519732	1
2/3,1/3,1-z	0.6666667	0.3333333	0.7480268	1

z= 0.2519732

1/3,2/3,1/4	0.333333333	0.666666667	0.251973233	1
2/3,1/3,3/4	0.666666667	0.333333333	0.748026767	1

Z'= 2

Order Parameter = Coupled

error 0 0 0.001973233

cr/ar= 1.51
cr/ar_ideal= 1.63
slightly compressed vs. ideal HCP

152b P_31_2_1
26 MTRETC10
a= 10.071
b= 10.071 b/a= 1
c= 25.922 c/a= 2.5739251
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 120 gamma= 120

Matrix Representation

1	-0.5	0	
0	0.8660254	0	
0	0	2.5739251	

a b c
1 1 2.5739251

Transformation to Reduced Cell

-1	0	-0.333333	0
0	1	0.333333	0.666667
0	0	-0.333333	0.166667
0	0	0	1

Det= 0.333333

Inverse Transformation

1	0	-1	0.166667
0	-1	-1	0.833333
0	0	-3	0.5
0	0	0	1

Det= 3

Matrix Representation

-1	-0.5	-0.5
0	0.866025404	0.288675135
0	0	-0.857975044

a b c
1 1 1.034144337

61.086313 61.086313 60
alpha beta gamma

Normalized Niggli Matrix

1	1	1.069454509
0.5	0.5	0.5

Daughter	152b	6	3	2
Ref. Lattice	FCC	48	1	48
			3	24
			(size)	(index)

Reduced Cell

Character	9 (hR)	… but very close to 1 (cF)	
Type	I		
b.b≥a.a	True	|b.c|≤|b.b/2	True
c.c≥b.b	True	|a.c|≤|a.a/2	True
2|D+E+F| ≤ A+B	N/A	|a.b|≤|a.a/2	True

Transformation to Conventional Cell

-1	1	1	0
1	-1	1	0
1	1	-1	0
0	0	0	1

Det= 4

Overall Transformation

0	0.5	-1	-0.166667
-0.5	0	-1	0.166667
-0.5	0.5	1	-0.5
0	0	0	1

Det= 0.75

12 neighbors within 8% of nearest
next neighbor 42% farther than nearest
sphere packing

Center of Mass Coordinates
b .2.

x,0,5/6	0.7146722	0	0.8333333	1
0,x,1/6	0	0.7146722	0.1666667	1
1-x,1-x,1/2	0.2853278	0.2853278	0.5	1

x= 0.7146722

0,0,0	0.048005556	0	-2	1
	0	-0.048005556	0	1
	-0.048005556	0.048005556	-1	1

Z'= 1

Order Parameter = LD3

error 0 -0.048005556 0

Tetragonal Crystal Structures (75-142)

141a I_41/a_m_d

27 FUZLUH

a= 14.5613
b= 14.5613 b/a= 1
c= 10.5074 c/a= 0.7215977
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

4 nearest neighbors
next neighbor 36% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	0.7215977

a	b	c
1	1	0.7215977
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

0	-0.5	0.5	0
0	-0.5	-0.5	1
1	0.5	0.5	-1
0	0	0	1

Det= 0.5

Inverse Transformation

0	1	1	0
-1	-1	0	1
1	-1	0	1
0	0	0	1

Det= 2

Center of Mass Coordinates

a -4m2 Origin Choice 2

0,3/4,1/8	0	0.75	0.125	1
1/2,3/4,3/8	0.5	0.75	0.375	1
1/2,1/4,5/8	0.5	0.25	0.625	1
0,1/4,7/8	0	0.25	0.875	1

Matrix Representation

0	-0.5	0.5
0	-0.5	-0.5
0.72159766	0.36079883	0.36079883

a	b	c
0.72159766	0.793836126	0.793836126
78.07854374	62.96720689	62.96720689
alpha	beta	gamma

Normalized Niggli Matrix

1	1.210239954	1.210239954
0.25	0.5	0.5

7/8,1/4,1/4	0.875	0.25	0.25	1
1/8,3/4,3/4	1.125	-0.25	0.75	1
	0.875	0.25	1.25	1
	1.125	0.75	0.75	1
error	0	0	0	

Daughter 141a
Ref. Lattice 141a

	|G|	Z	|G|/Z
	16	2	8
	16	2	8
		1	1
		(size)	(index)

Reduced Cell
Character 18 (tI)
Type I
b.b≥a.a True
c.c≥b.b True
2\|D+E+F\| ≤ A+B N/A

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

Z'= 2

c/a_conv= 0.72
c/a_ideal= 1.41
Very distorted diamond cubic.

Transformation to Conventional Cell

0	1	1	0
-1	-1	0	1
1	-1	0	1
0	0	0	1

Det= 2

Overall Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Order Parameter = GM1+

141a I_41/a_m_d

28 VAFWAA

a= 14.7313
b= 14.7313 b/a= 1
c= 10.5743 c/a= 0.7178117
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

4 nearest neighbors
next neighbor 35% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	0.7178117

a	b	c
1	1	0.7178117
90	90	90
alpha	beta	gamma

See #27 above.

See above.

Center of Mass Coordinates

a -4m2 Origin Choice 2

0,3/4,1/8	0	0.75	0.125	1
1/2,3/4,3/8	0.5	0.75	0.375	1
1/2,1/4,5/8	0.5	0.25	0.625	1
0,1/4,7/8	0	0.25	0.875	1

c/a_conv= 0.72
c/a_ideal= 1.41
Very distorted diamond cubic.

137a P_42/n_m_c

29 FUZTEZ

a= 8.5599
b= 8.5599 b/a= 1
c= 6.0179 c/a= 0.7030339
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

2 nearest neighbors
next neighbor 13% farther than nearest

Square packing of p-42m rods.

Matrix Representation

1	0	0
0	1	0
0	0	0.7030339

a	b	c
1	1	0.7030339
90	90	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates

a -4m2 (Origin Choice 1)

0,0,0	0	0	0	1

Molecular 3-fold axes

h 1

0,y,z	0	0.235	0.233	1
y,0,-z	0.235	0	-0.233	1
0,-y,z	0	-0.235	0.233	1
-y,0,-z	-0.235	0	-0.233	1
y=	0.235			
z=	0.233			

rod axis:

0	0	1

rod origin:

0	0	0

Transformation to orthogonal axes:

0		

Rotation about rod and rescaling:

0.707106781	-0.707106781	0	0
0.707106781	0.707106781	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.707106781	0.707106781	0	0
-0.707106781	0.707106781	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

-45 degrees

Rescaling parameter:

1

Matrix Representation

0.707106781	-0.707106781	0
0.707106781	0.707106781	0
0	0	0.703034

a	b	c
1	1	0.703034
90	90	90
alpha	beta	gamma

p-42m (#37)
2nd setting

a -42m

0,0,0	0	0	0	1	Z'= 1

f ..m

x,x,z	0.166170094	0.166170094	0.233	1
x,-x,-z	0.166170094	-0.166170094	-0.233	1
-x,-x,z	-0.166170094	-0.166170094	0.233	1
-x,x,-z	-0.166170094	0.166170094	-0.233	1
x=	0.166170094			
z=	0.233			

Daughter 137a
Rod 37a

	|G|	Z	|G|/Z
	16	2	8
	8	1	8
		2	1
		(size)	(index)

121a I_-4_2_m

30 ZZZKDW01

a= 6.4094
b= 6.4094 b/a= 1
c= 9.5586 c/a= 1.4913408
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

12 neighbors within 3% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	1.4913408

a	b	c
1	1	1.4913408
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

-1	0	0.5	0
0	-1	0.5	0
0	0	0.5	0
0	0	0	1

Det= 0.5

Inverse Transformation

-1	0	1	0
0	-1	1	0
0	0	2	0
0	0	0	1

Det= 2

Center of Mass Coordinates

a -4m2

0,0,0	0	0	0	1
1/2,1/2,1/2	0.5	0.5	0.5	1

Matrix Representation

-1	0	0.5
0	-1	0.5
0	0	0.745670422

a	b	c
1	1	1.027630467
119.1144824	119.1144824	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.056024378
-0.5	-0.5	0

0,0,0	0	0	0	1
	0	0	1	1

Z'= 1

Daughter 121a
Ref. Lattice FCC

	|G|	Z	|G|/Z
	8	1	8
	48	1	48
		1	6
		(size)	(index)

Reduced Cell
Character 15 (tI)
Type II
b.b≥a.a True
c.c≥b.b True
2\|D+E+F\| ≤ A+B Equal

… but close to singularity: 1 (cF)

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

-0.5	0.5	0	0
0	0	1	0
0.5	0.5	0	0
0	0	0	1

Det= 0.5

Order Parameter = GM5-

142a I_41/a_c_d

31 KUJSIR

a= 14.9351
b= 14.9351 b/a= 1
c= 30.2202 c/a= 2.0234347
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

12 neighbors within 1% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0
0	1	0
0	0	2.0234347

a	b	c
1	1	2.0234347
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

0.5	-0.5	0	0
0.5	0.5	-0.5	0.25
0	0	0.25	0.375
0	0	0	1

Det= 0.125

Inverse Transformation

1	1	2	-1
-1	1	2	-1
0	0	4	-1.5
0	0	0	1

Det= 8

Center of Mass Coordinates

a -4..

Origin Choice 2

0,1/4,3/8	0	0.25	0.375	1
0,3/4,5/8	0	0.75	0.625	1
1/2,1/4,5/8	0.5	0.25	0.625	1
1/2,3/4,3/8	0.5	0.75	0.375	1
1/2,3/4,7/8	0.5	0.75	0.875	1
1/2,1/4,1/8	0.5	0.25	0.125	1
0,3/4,1/8	0	0.75	0.125	1
0,1/4,7/8	0	0.25	0.875	1

Matrix Representation

0.5	-0.5	0
0.5	0.5	-0.5
0	0	0.505858682

a	b	c
0.707106781	0.707106781	0.71126156
119.8069547	119.8069547	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.011786012
-0.5	-0.5	0

0,0,0	0	0	0	1
	1	1	1	1
	1	0	1	1
	1	0	0	1
	2	1	2	1
	0	-1	-1	1
	0	0	-1	1
	1	1	2	1

Z'= 1

Daughter 142a
Ref. Lattice FCC

	|G|	Z	|G|/Z
	16	4	4
	48	1	48
		4	12
		(size)	(index)

Reduced Cell
Character 15 (tI)
Type II
b.b≥a.a True
c.c≥b.b True
2\|D+E+F\| ≤ A+B Equal

… but close to singularity: 1 (cF)

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

1	0	0	0
0	0	2	-0.75
0	-1	0	0.25
0	0	0	1

Det= 2

Order Parameter = W3

120c I_-4_c_2

32 YEMRIR

a= 9.0991
b= 9.0991 b/a= 1
c= 13.6601 c/a= 1.5012584
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

6 neighbors within 7% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0	
0	1	0	
0	0	1.5012584	

a	b	c	
1	1	1.5012584	
90	90	90	
alpha	beta	gamma	

Transformation to Reduced Cell

0.5	-0.5	0	0
0.5	0.5	0	0.5
0	0	0.5	0.25
0	0	0	1

Det= 0.25

Inverse Transformation

1	1	0	-0.5
-1	1	0	-0.5
0	0	2	-0.5
0	0	0	1

Det= 4

Matrix Representation

0.5	-0.5	0
0.5	0.5	0
0	0	0.750629183

a	b	c	
0.707106781	0.707106781	0.750629183	
90	90	90	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	1.126888341
0	0	0

Reduced Cell
Character 11 (tP) … but close to 3 (cP)
Type II
b.b≥a.a True |b.c|≤b.b/2 True
c.c≥b.b True |a.c|≤a.a/2 True
2|D+E+F| ≤ A+B True |a.b|≤a.a/2 True

	|G|	Z	|G|/Z
Daughter 120c	8	2	4
Ref. Lattice SC	48	1	48
		2	12
		(size)	(index)

Transformation to Conventional Cell

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Overall Transformation

1	1	0	-0.5
-1	1	0	-0.5
0	0	2	-0.5
0	0	0	1

Det= 4

Center of Mass Coordinates

c -4..

0,1/2,1/4	0	0.5	0.25	1	0,0,0	0	0	0	1	Z'= 1	Order Parameter = Coupled
0,1/2,3/4	0	0.5	0.75	1		0	0	1	1		
1/2,0,3/4	0.5	0	0.75	1		0	-1	1	1		
1/2,0,1/4	0.5	0	0.25	1		0	-1	0	1		

114a P_-4_21_c

33 ADAMAN08

a= 6.6397
b= 6.6397 b/a= 1
c= 8.9189 c/a= 1.3432685
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

12 neighbors within 3% of nearest
next neighbor 38% farther than nearest
sphere packing

Matrix Representation

1	0	0	
0	1	0	
0	0	1.3432685	

a	b	c	
1	1	1.3432685	
90	90	90	
alpha	beta	gamma	

Transformation to Reduced Cell

0.5	-0.5	0.5	0
0.5	0.5	-0.5	0
-0.5	0.5	0.5	0
0	0	0	1

Det= 0.5

Inverse Transformation

1	1	0	0
0	1	1	0
1	0	1	0
0	0	0	1

Det= 2

Matrix Representation

0.5	-0.5	0.5
0.5	0.5	-0.5
-0.671634261	0.671634261	0.671634261

a	b	c	
0.975239755	0.975239755	0.975239755	
92.9475839	118.3130554	118.3130554	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	1
-0.051422355	-0.474288823	-0.474288823

Reduced Cell
Character 7 (tI) … but close to singularity: 1 (cF)
Type II
b.b≥a.a True |b.c|≤b.b/2 True
c.c≥b.b True |a.c|≤a.a/2 True
2|D+E+F| ≤ A+B Equal |a.b|≤a.a/2 True

	|G|	Z	|G|/Z
Daughter 114a	8	2	4
Ref. Lattice FCC	48	1	48
		2	12
		(size)	(index)

Transformation to Conventional Cell

0	0	2	0
1	1	1	0
-1	1	1	0
0	0	0	1

Det= 4

Overall Transformation

-0.5	0.5	0	0
0	0	1	0
0.5	0.5	0	0
0	0	0	1

Det= 0.5

Center of Mass Coordinates

a -4..

0,0,0	0	0	0	1	0,0,0	0	0	0	1	Z'= 1	Order Parameter = Coupled
1/2,1/2,1/2	0.5	0.5	0.5	1		1	1	1	1		

114b P_-4_21_c

34 GERHOA

a= 10.0441
b= 10.0441 b/a= 1
c= 12.4722 c/a= 1.2417439
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

12 neighbors within 7% of nearest
next neighbor 32% farther than nearest
sphere packing

See above.

Matrix Representation

1	0	0	
0	1	0	
0	0	1.2417439	

a	b	c	
1	1	1.2417439	
90	90	90	
alpha	beta	gamma	

Transformation to Reduced Cell

0.5	-0.5	0.5	0
0.5	0.5	-0.5	0
-0.5	0.5	0.5	0.5
0	0	0	1

Det= 0.5

Inverse Transformation

1	1	0	0
0	1	1	-0.5
1	0	1	-0.5
0	0	0	1

Det= 2

Matrix Representation

0.5	-0.5	0.5
0.5	0.5	-0.5
-0.620871955	0.620871955	0.620871955

a	b	c	
0.941000523	0.941000523	0.941000523	
97.43078797	115.8066616	115.8066616	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	1
-0.129328454	-0.435335773	-0.435335773

See #33 above.

Along tetragonal path from FCC to BCC.
Closer to FCC than BCC.

Center of Mass Coordinates

b -4..

0,0,1/2	0	0	0.5	1	0,0,0	0	0	0	1		
1/2,1/2,0	0.5	0.5	0	1		1	0	0	1		

88a I_41/a

35 KANGUB01

a= 7.1984
b= 7.1984 b/a= 1
c= 28.582 c/a= 3.9706046
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

8 neighbors within 12% of nearest
next neighbor 41% farther than nearest
sphere packing

Matrix Representation

1	0	0	
0	1	0	
0	0	3.9706046	

a	b	c	
1	1	3.9706046	
90	90	90	
alpha	beta	gamma	

Transformation to Reduced Cell

1	0	-0.5	0
0	1	-0.5	-0.5
0	0	0.5	0
0	0	0	1

Det= 0.5

Inverse Transformation

1	0	1	0
0	1	1	0.5
0	0	2	0
0	0	0	1

Det= 2

Matrix Representation

1	0	-0.5
0	1	-0.5
0	0	1.985302289

a	b	c	
103.7243738	103.7243738	90	
alpha	beta	gamma	

Normalized Niggli Matrix

1	1	4.44142518
-0.5	-0.5	0

Reduced Cell
Character 15 (tI)
Type II
b.b≥a.a True |b.c|≤b.b/2 True
c.c≥b.b True |a.c|≤a.a/2 True
2|D+E+F| ≤ A+B Equal |a.b|≤a.a/2 True

	|G|	Z	|G|/Z
Daughter 88a	16	4	4
Ref. Lattice 141a	16	2	8
		2	2
		(size)	(index)

Transformation to Conventional Cell

1	0	1	0
0	1	1	0
0	0	2	0
0	0	0	1

Det= 2

Overall Transformation

1	0	0	0
0	1	0	0.5
0	0	1	0
0	0	0	1

Det= 1

Center of Mass Coordinates

a -4..

0,1/4,1/8	0	0.25	0.125	1	1/8,7/8,1/4	0.125	0.875	0.25	1	Z'= 2	Order Parameter = GM3+
1/2,1/4,3/8	0.5	0.25	0.375	1	7/8,1/8,3/4	0.875	1.125	0.75	1		
1/2,3/4,5/8	0.5	0.75	0.625	1		1.125	1.875	1.25	1		
0,3/4,7/8	0	0.75	0.875	1		0.875	2.125	1.75	1		

c/a_conv= 3.97
c/a_ideal= 1.41
Very distorted diamond cubic.

88f I_41/a

36 LUFYEQ

a= 15.66931
b= 15.66931 b/a= 1
c= 19.5592 c/a= 1.2482486
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

1 nearest neighbor
next neighbor 33% farther than nearest
dimer packing

Matrix Representation

1	0	0	
0	1	0	
0	0	1.2482486	

a	b	c	
1	1	1.2482486	
90	90	90	
alpha	beta	gamma	

Transformation to Reduced Cell

0.5	0.5	-0.5	0.25
0.5	-0.5	0.5	0.25
0.5	-0.5	-0.5	0.25
0	0	0	1

Det= 0.5

Inverse Transformation

1	1	0	-0.5
1	0	-1	0
0	1	-1	0
0	0	0	1

Det= 2

Matrix Representation

0.5	0.5	-0.5
0.5	-0.5	0.5
0.624124324	-0.624124324	-0.624124324

a	b	c	
0.943149602	0.943149602	0.943149602	
97.13384882	115.9703615	115.9703615	
alpha	beta	gamma	

Center of Mass Coordinates

f 1

a	x,y,z	0.0519571	0.0932353	0.3109161	1		-0.3548076	-0.258959	-0.21768084	1	Z'= 8
b	1/2-x,1-y,1.	0.4480429	0.9067647	0.8109161	1		0.8548076	-0.36287324	0.0958486	1	
c	3/4-y,1/4+x	0.6567647	0.3019571	0.5609161	1		0.45872184	0.0958486	-0.258959	1	
d	3/4+y,3/4-x	0.8432353	0.6980429	1.0609161	1		1.04127816	-0.21768084	-0.36287324	1	
e	1-x,1-y,1-z	0.9480429	0.9067647	0.6890839	1		1.3548076	0.258959	0.21768084	1	
f	1/2+x,y,1/2	0.5519571	0.0932353	0.1890839	1		0.1451924	0.36287324	-0.0958486	1	
g	1/4+y,3/4-x	0.3432353	0.6980429	0.4390839	1		0.54127816	-0.0958486	0.258959	1	
h	1/4-y,1/4+x	0.1567647	0.3019571	-0.060916	1		-0.04127816	0.21768084	0.36287324	1	
b	1/2+x,1/2+	0.5519571	0.5932353	0.8109161	1		0.6451924	-0.258959	-0.21768084	1	
a	1-x,1/2-y,z	0.9480429	0.4067647	0.3109161	1		0.8548076	0.63712676	0.0958486	1	
d	1/4-y,3/4+x	0.1567647	0.8019571	1.0609161	1		0.45872184	-0.9041514	-0.258959	1	
c	1/4+y,1/4-x	0.3432353	0.1980429	0.5609161	1		0.04127816	-0.21768084	-0.36287324	1	
f	1/2-x,1/2-y	0.4480429	0.4067647	0.1890839	1	x,y,z	0.3548076	0.258959	0.21768084	1	
e	x,1/2+y,1-z	0.0519571	0.5932353	0.6890839	1		0.1451924	-0.63712676	-0.0958486	1	
h	3/4+y,1/4-x	0.8432353	0.1980429	-0.060916	1		0.54127816	0.9041514	0.258959	1	
g	3/4-y,3/4+x	0.6567647	0.8019571	0.4390839	1		0.95872184	0.21768084	0.36287324	1	

x= 0.0519571
y= 0.0932353
z= 0.3109161

dimers:

Dimer Coordinates (e), 2.. WP Symmetry ensures C2 dimer symmetry
Slightly distorted C2v dimers

Transformation to Reduced Cell

0.5	0.5	-0.5	0.25
0.5	-0.5	0.5	0.25
0.5	-0.5	-0.5	0.25
0	0	0	1

Det= 0.5

Inverse Transformation

1	1	0	-0.5
1	0	-1	0
0	1	-1	0
0	0	0	1

Det= 2

Matrix Representation

0.5	0.5	-0.5
0.5	-0.5	0.5
0.624124324	-0.624124324	-0.624124324

	a	b	c
	0.943149602	0.943149602	0.943149602
	97.13384882	115.9703615	115.9703615
	alpha	beta	gamma

Normalized Niggli Matrix

1	1	1
-0.124187698	-0.437906151	-0.437906151

		|G|	Z	|G|/Z
Daughter	88f	8	8	1
C2 Dimers	88e	8	4	2
Ref. Lattice	141e	16	4	4
		1	1	2
			(size)	(index)

Reduced Cell

Character	7 (tI)
Type	II
b.b≥a.a	True
c.c≥b.b	True
2|D+E+F| ≤ A+B	Equal

|b.c|≤b.b/2	True	
|a.c|≤a.a/2	True	
|a.b|≤a.a/2	True	

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

0	0	-1	0.25
0	1	0	-0.25
1	0	0	-0.25
0	0	0	1

Det= 1

Dimer Center of Mass Coordinates

		e 2..	Origin Choice 2			
a	0,1/4,z	0	0.25	0.3109161	1	
b		0.5	0.75	0.8109161	1	
c		0.5	0.25	0.5609161	1	
d		0	0.75	1.0609161	1	
e		0	0.75	0.6890839	1	
f		0.5	0.25	0.1890839	1	
g		0.5	0.75	0.4390839	1	
h		0	0.25	-0.060916	1	
		z= 0.3109161				

	-0.25	-0.31091612	-0.06091612	1
3/4,2/3,11/	0.75	-0.31091612	-0.06091612	1
1/4,11/12,2	0.25	-0.06091612	-0.31091612	1
	0.25	-1.06091612	-0.31091612	1
	0.25	-0.68908388	0.06091612	1
1/4,1/3,1/1:	0.25	0.31091612	0.06091612	1
3/4,1/12,1/	0.75	0.06091612	0.31091612	1
	-0.25	0.06091612	0.31091612	1
error	0	0.022417213	-0.022417213	

Z' = 4

Order Parameter = X5+

quads:

Quadramer Coordinates (a), -4.. WP Symmetry ensures S4 quadramer symmetry

4 equidistant nearest neighbors
next neighbor >60% further
sphere packing (of quadramers)

Quadramer Center of Mass Coordinates

		a -4..	Origin Choice 2			
ah	0,1/4,1/8	0	0.25	0.125	1	
bg	1/2,3/4,5/8	0.5	0.75	0.625	1	
cf	1/2,1/4,3/8	0.5	0.25	0.375	1	
de	0,3/4,7/8	0	0.75	0.875	1	

		|G|	Z	|G|/Z
Daughter	88f	8	8	1
C2 Dimers	88e	8	4	2
S4 Quadramers	88a	8	2	4
Ref. Lattice	227a	48	2	24
		1	1	6
			(size)	(index)

c/a_conv= 1.25
c/a_ideal= 1.41
Somewhat compressed diamond cubic.

Overall Transformation

0.5	0.5	0	0.5
-0.5	0.5	0	0.5
0	0	1	0
0	0	0	1

Det= 1

Order Parameter = GM4+

Orthorhombic Crystal Structures (16-74)

62c P_n_m_a
37 GUTCED
a= 11.47068
b= 12.64188 b/a= 1.1021038
c= 12.51698 c/a= 1.0912152
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

Matrix Representation

1	0	0
0	1.1021038	0
0	0	1.0912152

	a	b	c
	1	1.1021038	1.0912152
	90	90	90
	alpha	beta	gamma

2 nearest neighbors
next neighbor 10% farther than nearest

Square packing of p1121/m rods.

Transformation to Rod Coordinates

0	1	0	0.5
0	0	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

0	0	1	0
1	0	0	-0.5
0	1	0	0
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.957292823	0	0	0
0	1.04612449	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.044612449	0	0	0
0	0.957292823	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0	1.044612449	0
0	0	1.102104
1.044612449	0	0

	a	b	c
	1.044612449	1.044612449	1.102104
	90	90	90
	alpha	beta	gamma

p1121/m (#12)

		|G|	Z	|G|/Z
Daughter	62c	8	4	2
Rod	12b	4	2	2
			2	1
			(size)	(index)

Center of Mass Coordinates

		c .m.				
i	x,1/4,z	0.3286569	0.25	-0.013779	1	
ii	1-x,3/4,1-z	0.6713431	0.75	1.013779	1	
	1/2-x,3/4,1.	0.1713431	0.75	0.486221	1	
	1/2+x,1/4,1	0.8286569	0.25	0.513779	1	
		x= 0.3286569				
		z= -0.013779				

rod axis:
0 1 0
rod origin:
0.5 0 0
Transformation to orthogonal axes:
0

rotation angle:
0 degrees
Rescaling parameter:
0.957292823

		b m			
x,y,1/4	-0.014393677	-0.164025564	0.25	1	Z'= 2
-x,-y,3/4	1.059006126	0.164025564	0.75	1	
	0.507912547	-0.314620847	0.75	1	
	0.536699901	0.314620847	0.25	1	
error	0	0	0		

Molecular 3-fold axes

	c .m.			
i	0.4309	0.25	-0.2415	1
i	0.5287	0.25	0.1508	1
	d 1			
i	0.177	0.4492	0.018	1
i	0.177	0.0508	0.018	1
	c .m.			
ii	0.4713	0.75	-0.1508	1
ii	0.5691	0.75	0.2415	1
	d 1			
ii	0.823	0.5508	-0.018	1
ii	0.823	0.9492	-0.018	1

	b m			
	-0.252273906	-0.066148934	0.25	1
x,y,1/4	0.157527557	0.027474304	0.25	1
	b m			
-x,-y,3/4	-0.157527557	-0.027474304	0.75	1
	0.252273906	0.066148934	0.75	1

62c P_n_m_a
38 JEYSEL
a= 10.0621
b= 16.3473 b/a= 1.624641
c= 18.0792 c/a= 1.7967621
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

Matrix Representation

1	0	0
0	1.624641	0
0	0	1.7967621

	a	b	c
	1	1.624641	1.7967621
	90	90	90
	alpha	beta	gamma

2 nearest neighbors
next neighbor 12% farther than nearest

See above.

Transformation to Rod Coordinates

0	1	0	0
0	0	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

0	0	1	0
1	0	0	0
0	1	0	0
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.746027282	0	0	0
0	1.340433552	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.340433552	0	0	0
0	0.746027282	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0	1.340433552	0
0	0	1.624641
1.340433552	0	0

	a	b	c
	1.340433552	1.340433552	1.624641
	90	90	90
	alpha	beta	gamma

p1121/m (#12)

See # 37 above.

Center of Mass Coordinates

		c .m.				
i	x,1/4,z	-0.06938	0.25	-0.030205	1	
	1/2-x,3/4,1.	0.5693802	0.75	0.469795	1	
ii	1-x,3/4,1-z	1.0693802	0.75	1.030205	1	
	1/2+x,1/4,1	0.4306198	0.25	0.530205	1	
		x= -0.06938				
		z= -0.030205				

rod axis:
0 1 0
rod origin:
0 0 0
Transformation to orthogonal axes:
0

rotation angle:
0 degrees
Rescaling parameter:
0.746027282

		b m			
x,y,1/4	-0.040487816	-0.051759486	0.25	1	Z'= 2
-x,-y,3/4	0.62972896	0.424773127	0.75	1	
	1.380921368	0.797786768	0.75	1	
	0.710704592	0.321254155	0.25	1	
error	0	0	0		

Molecular 3-fold axes

	c .m.			
i	0.3077	0.25	-0.0354	1
i	-0.1829	0.25	0.1574	1
	d 1			
i	-0.1771	0.0646	-0.1282	1
i	-0.1771	0.4354	-0.1282	1
	c .m.			
ii	-0.3077	0.75	0.0354	1

	b m			
	-0.047451348	0.229552595	0.25	1
x,y,1/4	0.210984241	-0.13644839	0.25	1
	b m			
	0.047451348	-0.229552595	0.75	1

ii 0.1829 0.75 -0.1574 1 — -x,-y,3/4 -0.210984241 0.13644839 0.75 1
d 1
ii 0.1771 0.9354 0.1282 1
ii 0.1771 0.5646 0.1282 1

62c P_n_m_a
39 RIMMOP

a=	10.33609		
b=	15.0811	b/a=	1.459072
c=	16.6321	c/a=	1.6091288
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

2 nearest neighbors
next nearest neighbors are not coplanar
next neighbor 17% farther than nearest

See above.

Matrix Representation

1	0	0
0	1.459072	0
0	0	1.6091288
a	b	c
1	1.459072	1.6091288
90	90	90
alpha	beta	gamma

Transformation to Rod Coordinates

0	1	0	0.5
0	0	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

0	0	1	0
1	0	0	-0.5
0	1	0	0
0	0	0	1

Det= 1

rod axis: 0 1 0
rod origin: 0.5 0 0
Transformation to orthogonal axes: 0

Rotation about rod and rescaling:

0.788323726	0	0	0
0	1.268514403	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.268514403	0	0	0
0	0.788323726	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle: 0 degrees
Rescaling parameter: 0.788323726

Matrix Representation

0	1.268514403	0
0	0	1.459072
1.268514403	0	0
a	b	c
1.268514403	1.268514403	1.459072
90	90	90
alpha	beta	gamma

See # 37 above.

p1121/m (#12)

Center of Mass Coordinates

	c .m.				
i	x,1/4,z	0.1867586	0.25	0.4677994	1
	1/2-x,3/4,1.	0.3132414	0.75	0.9677994	1
ii	1-x,3/4,1-z	0.8132414	0.75	0.5322006	1
	1/2+x,1/4,1	0.6867586	0.25	0.0322006	1
	x=	0.1867586			
	z=	0.4677994			

b	m			
x,y,1/4	0.593410245	-0.246935632	0.25	1
	1.227667446	-0.14722623	0.75	1
-x,1-y,3/4	0.675104158	0.246935632	0.75	1
	0.040846957	0.14722623	0.25	1

Z'= 2

Molecular 3-fold axes

	c .m.				
i	x,1/4,z	0.0266	0.25	0.4729	1
ii	1-x,3/4,1-z	-0.0266	0.75	0.5271	1
	c .m.				
i	x,1/4,z	0.2488	0.25	0.5612	1
ii	1-x,3/4,1-z	0.7512	0.75	0.4388	1
	d 1				
i	x,y,z	0.2371	0.1593	0.4189	1
i	x,1/2-y,z	0.2371	0.3407	0.4189	1
ii	1-x,1/2+y,1	0.7629	0.6593	0.5811	1
ii	1-x,1-y,1-z	0.7629	0.8407	0.5811	1

b	m			
	0.599880461	-0.373192452	0.25	1
	0.668633942	-0.415131274	0.75	1
b	m			
	0.711890283	-0.19802692	0.25	1
	0.55662412	0.19802692	0.75	1

64d,f C_m_c_a Renamed Cmce
40 METHANEiii

a=	11.7079		
b=	8.1893	b/a=	0.6994679
c=	8.1842	c/a=	0.6990323
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

Not from the CSD. See Neuman '03

Matrix Representation

1	0	0
0	0.6994679	0
0	0	0.6990323
a	b	c
1	0.6994679	0.6990323
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

0	0	0.25	0.25
0	-0.5	0.25	0
0.5	0	-0.25	0
0	0	0	1

Det= 0.0625

Inverse Transformation

2	0	2	-0.5
2	-2	0	-0.5
4	0	0	-1
0	0	0	1

Det= 16

Matrix Representation

0	0	0.25
0	-0.34973394	0.17486697
0.349516139	0	-0.174758069
a	b	c
0.349516139	0.34973394	0.35159471
119.8250837	119.8046299	90
alpha	beta	gamma

Normalized Niggli Matrix

1	1.001246692	1.01192936
-0.500623346	-0.5	0

Daughter	64d,f		
Ref. Lattice	FCC		

|G|	Z	|G|/Z
8	8	1
48	1	48
	8	48
	(size)	(index)

Reduced Cell
Character 42 (oI) … but close to singularity: 1 (cF)
Type II

b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	Equal	|a.b|≤a.a/2	True

sphere packing

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

0	1	1	0
2	0	0	-0.5
0	1	-1	0
0	0	0	1

Det= 4

Order Parameter = Coupled

Center of Mass Coordinates

d: 2 nearest neighbors
12 neighbors within 9%
next neighbor >46% further

d 2..										
x,0,0	0.24982	0	0	1	0,0,0	-0.00036	-0.00036	-0.00072	1	Z'= 1
1-x,1/2,1/2	0.75018	0.5	0.5	1		2.00036	0.00036	2.00072	1	
1-x,0,0	0.75018	0	0	1		1.00036	1.00036	2.00072	1	
x,1/2,1/2	0.24982	0.5	0.5	1		0.99964	-1.00036	-0.00072	1	
1/2+x,1/2,0	0.74982	0.5	0	1		0.99964	-0.00036	1.99928	1	
1/2-x,0,1/2	0.25018	0	0.5	1		1.00036	0.00036	0.00072	1	
1/2-x,1/2,0	0.25018	0.5	0	1		0.00036	-0.99964	0.00072	1	
1/2+x,0,1/2	0.74982	0	0.5	1		1.99964	0.99964	1.99928	1	
x=	0.24982									
					error	0.00036	0.00036	0.00072		

f: 2 nearest neighbors
12 neighbors within 9%
next neighbor >34% further

Sphere packing

f m..									
0,y,z	0	0.22962	0.26968	1		0.03936	-0.95924	-1	1
0,1/2-y,1/2	0	0.27038	0.76968	1		1.03936	-1.04076	-1	1
0,1/2+y,1/2	0	0.72962	0.23032	1		-0.03936	-1.95924	-1	1
0,1-y,1-z	0	0.77038	0.73032	1		0.96064	-2.04076	-1	1
1/2,1/2+y,z	0.5	0.72962	0.26968	1		1.03936	-0.95924	1	1
1/2,1-y,1/2	0.5	0.77038	0.76968	1		2.03936	-1.04076	1	1
1/2,y,1/2-z	0.5	0.22962	0.23032	1		0.96064	0.04076	1	1
1/2,1/2-y,1-	0.5	0.27038	0.73032	1		1.96064	-0.04076	1	1
y=	0.22962								
z=	0.26968				error	0.03936	0.04076	0	

19a P_21_21_21
41 MZNMOX10

a=	7.48115		
b=	7.67315	b/a=	1.0256645
c=	29.425	c/a=	3.9332188
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

4 neighbors within 3% of nearest (coplanar)
next neighbor 13% farther than nearest
planar packing

Matrix Representation

1	0	0
0	1.0256645	0
0	0	3.9332188
a	b	c
1	1.0256645	3.9332188
90	90	90
alpha	beta	gamma

Transformation to Planar Coordinates

1	0	0	-0.065579
0	1	0	0.067456
0	0	1	0.122842
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0.065579
0	1	0	-0.067456
0	0	1	-0.122842
0	0	0	1

Det= 1

plane normal: 0 0 1
plane origin: -0.065579 0.067456 0.122842
Transformation to orthogonal axes: 0

Rotation about plane normal and rescaling:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle: 0 degrees
Rescaling parameter: 1 1.012750958

Matrix Representation

1	6.28296E-17	0
0	1.025664503	0
0	0	3.933219
a	b	c
1	1.025664503	3.933219
90	90	90
alpha	beta	gamma

p1 (#1)
distorted p4mm (#11)
S4 (-4) when accounting for 3rd dimension

		|G|	Z	|G|/Z
Daughter	P_21_21_2	4	4	1
Plane	p1	1	1	1
			4	1
			(size)	(index)

Center of Mass Coordinates

	a 1				
i	x,y,z	-0.065579	0.0674563	0.1228419	1
	1/2-x,1-y,1.	0.5655794	0.9325438	0.6228419	1
	1-x,1/2+y,1	1.0655794	0.5674563	0.3771581	1
	1/2+x,1/2-y	0.4344206	0.4325438	0.8771581	1
	x=	-0.065579			
	y=	0.0674563			
	z=	0.1228419			

0,0,0	0	0	0	1	Z'= 1
x,y,z	-0.213620625	-0.06335625	-0.027342	1	
x,y,z	0.141979375	0.13474375	-0.041342	1	
x,y,z	-0.045120625	0.13914375	0.052158	1	
x,y,z	0.130879375	-0.19945625	0.017458	1	

Molecular 3-fold axes

	a 1				
i	x,y,z	-0.2792	0.0041	0.0955	1
i	x,y,z	0.0764	0.2022	0.0815	1
i	x,y,z	-0.1107	0.2066	0.175	1
i	x,y,z	0.0653	-0.132	0.1403	1

60c,d P_b_c_n

42 YIMWEW

a=	24.4809		
b=	10.9912	b/a=	0.4489704
c=	11.2429	c/a=	0.4592519
alpha=	90	alpha=	90
beta=	90	beta=	90
gamma=	90	gamma=	90

Matrix Representation

1	0	0	
0	0.4489704	0	
0	0	0.4592519	
a	b	c	
1	0.4489704	0.4592519	
90	90	90	
alpha	beta	gamma	

Transformation to Reduced Cell

0.166667	0.166667	-0.166667	0
0.5	-0.5	0	-0.25
0	0	-0.5	0.25
0	0	0	1

Det= 0.083333

Inverse Transformation

3	1	-1	0.5
3	-1	-1	0
0	0	-2	0.5
0	0	0	1

Det= 12

Matrix Representation

0.166666667	0.166666667	-0.166666667
0.224485211	-0.224485211	0
0	0	-0.229625953
a	b	c
0.279591466	0.279591466	0.283735539
110.4967722	110.4967722	106.8167033
alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.029863465
-0.355344565	-0.355344565	-0.289310869

Daughter 60c,d
Ref. Lattice BCC

	|G|	Z	|G|/Z
	8	12	0.666667
	48	1	48
		12	72
		(size)	(index)

Reduced Cell

Character	16 (oF)	… but close to 5 (cI)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	Equal	|a.b|≤a.a/2	True

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

0	-1	-1	0
0	1	-1	0.5
3	0	0	0
0	0	0	1

Det= 6

Center of Mass Coordinates

c 2 nearest neighbors — c .2.

8 neighbors within 5% of nearest	0,y,1/4	0	-0.187538	0.25	1
next neighbor 11% farther than nearest	1/2,1/2-y,3.	0.5	0.687538	0.75	1
	0,1-y,3/4	0	1.187538	0.75	1
	1/2,1/2+y,1	0.5	0.312462	0.25	1

y= -0.187538

d 1 nearest neighbor — d 1

7 neighbors within 5% of nearest	x,y,z	0.1688182	0.2974947	0.206184	1
9 neighbors within 8% of nearest	1/2-x,1/2-y	0.3311818	0.2025053	0.706184	1
next neighbor >11% farther than nearest	1-x,y,1/2-z	0.8311818	0.2974947	0.293816	1
	1/2+x,1/2-y	0.6688182	0.2025053	0.793816	1
	1-x,1-y,1-z	0.8311818	0.7025053	0.793816	1
Sphere packing	1/2+x,1/2+	0.6688182	0.7974947	0.293816	1
	x,1-y,1/2+z	0.1688182	0.7025053	0.706184	1
	1/2-x,1/2+y	0.3311818	0.7974947	0.206184	1

x= 0.1688182
y= 0.2974947
z= 0.206184

0,0,0

0.062462	-0.062462	0	1	Z'= 1
1.937538	0.062462	-1	1	
0.937538	-1.937538	-1	1	
2.062462	0.937538	0	1	
1.097765367	0.002776033	0.087632	1	
0.989866633	0.084855967	-0.912368	1	
2.997223967	1.902234633	-0.087632	1	
1.915144033	1.010133367	-1.087632	1	
2.902234633	0.997223967	-1.087632	1	
3.010133367	0.915144033	-0.087632	1	
1.002776033	-0.902234633	-0.912368	1	
2.084855967	-0.010133367	0.087632	1	

Order Parameter = Coupled

Monoclinic Crystal Structures (3-15)

15e *A2/a*

43 BOGMEP

a=	19.4179		
b=	9.7886	b/a=	0.5041019
c=	22.7929	c/a=	1.1738087
alpha=	90	alpha=	90
beta=	116.083	beta=	116.083
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.516092	
0	0.5041019	0	
0	0	1.0542658	
a	b	c	
1	0.5041019	1.1738087	
90	116.083	90	
alpha	beta	gamma	

Transformation to Rod Coordinates

1	-0.516081	0	0.25
0	0	1	0.25689
0	-1	0	0.5
0	0	0	1

Det= 1

Inverse Transformation

1	0	-0.516081	0.008041
0	0	-1	0.5
0	1	0	-0.25689
0	0	0	1

Det= 1

Rotation about rod and rescaling:

1.026221172	-0.032039118	0	0
0.030393135	0.973499922	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.973499922	0.032039118	0	0
-0.030393135	1.026221172	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

1.026221494	-0.032028812	0	
0	0	0.504102	
-0.032042441	-1.026327633	0	
a	b	c	
1.026721614	1.026827276	0.504102	
90	90	90	
alpha	beta	gamma	

Daughter 15e
Rod 37a

	|G|	Z	|G|/Z
	4	2	2
	8	1	8
		2	4
		(size)	(index)

2 nearest neighbors
next neighbor 10.5% farther than nearest

p112 (#8)
… but close to p-4m2 (#37)

Hexagonal packing of p-4m2 rods.

Center of Mass Coordinates

e 2

i	1/4,y,1/2	0.25	0.2568903	0.5	1
	1/4,1/2+y,(	0.25	0.7568903	0	1
	3/4,1/2-y,0	0.75	0.2431097	0	1
	3/4,1-y,1/2	0.75	0.7431097	0.5	1

y= 0.2568903

rod axis: 0 1 0

rod origin: 0.25 0.25689 0.5

Transformation to orthogonal axes:
-0.516081

rotation angle:
-1.788220892 degrees

Rescaling parameter:
1.026721188

a -4m2

0,0,0	0	0	0	1	Z'= 1
	0.267221992	0.505267925	0.5	1	
	0.753971953	0.490071358	-0.013781	1	
	0.486749961	-0.015196567	0.486219	1	
error	0	0	0		

Molecular 3-fold axes

f 1

i	1/2-x,y,1-z	0.3347	0.1504	0.5517	1
i	x,y,z	0.1653	0.1504	0.4483	1
i		0.2219	0.3791	0.5538	1
i		0.2781	0.3791	0.4462	1

f m

x,-x,-z	0.054824689	-0.054819002	-0.10649	1
-x,x,-z	-0.054824689	0.054819002	-0.10649	1
-x,-x,z	-0.056108434	-0.053512782	0.12221	1
x,x,z	0.056108434	0.053512782	0.12221	1

x= 0.054816227
z= 0.11435

error	0.001292207	-0.001303445	0.00786	

15e C2/c

44 MSISUL10

a=	9.3821		
b=	16.5132	b/a=	1.760075
c=	10.58411	c/a=	1.1281174
alpha=	90	alpha=	90
beta=	107.1717	beta=	107.1717
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.333061	
0	1.760075	0	
0	0	1.0778308	
a	b	c	
1	1.760075	1.1281174	
90	107.1717	90	
alpha	beta	gamma	

Transformation to Rod Coordinates

1	0	0	0
0	1	0	0.5
0.261707	0	1	0.5
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	-0.5
-0.261707	0	1	-0.5
0	0	0	1

Det= 1

Rotation about rod and rescaling:

1.357273748	0	0	0
0	0.736771047	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.736771047	0	0	0
0	1.357273748	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

1.238967834	0	-0.333061	
0	1.296772327	0	
0.382853985	0	1.077831	
a	b	c	
1.296772327	1.296772327	1.128117	
90	90	90	
alpha	beta	gamma	

Daughter 15e
Rod 22b

	|G|	Z	|G|/Z
	4	2	2
	8	2	4
		1	2
		(size)	(index)

2 nearest neighbors
next neighbor 19% farther than nearest

pmcm (#22)

Hexagonal packing of pmcm rods.

Center of Mass Coordinates

e 2

	0,y,1/4	0	0.8926227	0.25	1
i	0,1-y,3/4	0	0.1073773	0.75	1
	1/2,1/2+y,1	0.5	0.3926227	0.25	1
	1/2,1/2-y,3.	0.5	0.6073773	0.75	1

y= 0.8926227

rod axis: 0 0 1

rod origin: 0 0.5 0.5

Transformation to orthogonal axes:
0.261707

rotation angle:
0 degrees

Rescaling parameter:
1.357273748

b m2m

0,-y,3/4	0	0.532896473	-0.25	1	Z'= 2
0,y,1/4	0	-0.532896473	0.25	1	
	0.368385523	-0.145740401	-0.380853	1	
	0.368385523	0.145740401	0.119147	1	

Molecular 3-fold axes

f 1

i	-0.0026	0.1801	0.9088	1
i	0.0026	0.1801	0.5912	1

f 1

i	-0.1872	0.0356	0.6989	1
i	0.1872	0.0356	0.8011	1

d m

0,y,1/2-z	-0.001915605	-0.434191872	0.40948	1
0,y,z	0.001915605	-0.434191872	0.09052	1
error	0.001915605	0	0	

e m

-x,y,1/4	-0.13792354	-0.630317929	0.247892	1
x,y,1/4	0.13792354	-0.630317929	0.252108	1
error	0	0	0.002108	

15e C2/c

45 TMGEHS10

a=	9.4225		
b=	16.7798	b/a=	1.7808225
c=	10.7085	c/a=	1.1364818
alpha=	90	alpha=	90
beta=	107.943	beta=	107.943
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.350117	
0	1.7808225	0	
0	0	1.0812073	
a	b	c	
1	1.7808225	1.1364818	
90	107.943	90	
alpha	beta	gamma	

See #44 above.

2 nearest neighbors

next neighbor 19% farther than nearest
rod packing

See above.

Center of Mass Coordinates

		e	2	
0,y,1/4	0	0.8945	0.25	1
0,1-y,3/4	0	0.1055	0.75	1
1/2,1/2+y,1	0.5	0.3945	0.25	1
1/2,1/2-y,3/4	0.5	0.6055	0.75	1

y= 0.8945

15e C2/c

46 TMSNHS10

a= 9.7726
b= 17.3516 b/a= 1.7755357
c= 10.9585 c/a= 1.1213495
alpha= 90 alpha= 90
beta= 108.984 beta= 108.984
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.36478
0	1.7755357	0
0	0	1.0603587

	a	b	c
	1	1.7755357	1.1213495
	90	108.984	90
	alpha	beta	gamma

See #44 above.

2 nearest neighbors
next neighbor 21% farther than nearest
rod packing

See above.

Center of Mass Coordinates

		e	2	
0,y,1/4	0	0.1023143	0.25	1
0,1-y,3/4	0	0.8976857	0.75	1
1/2,1/2+y,1	0.5	0.6023143	0.25	1
1/2,1/2-y,3/4	0.5	0.3976857	0.75	1

y= 0.1023143

15e C2/c

47 RASDOE

a= 20.0104
b= 10.1162 b/a= 0.5055471
c= 19.3224 c/a= 0.9656179
alpha= 90 alpha= 90
beta= 120.132 beta= 120.132
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.484734
0	0.5055471	0
0	0	0.8351351

	a	b	c
	1	0.5055471	0.9656179
	90	120.132	90
	alpha	beta	gamma

Transformation to Reduced Cell

0	-0.5	-0.5	0.25
-1	-0.5	-0.5	0.75
0	0	-1	0.5
0	0	0	1

Det= 0.5

Inverse Transformation

1	-1	0	0.5
-2	0	1	0
0	0	-1	0.5
0	0	0	1

Det= 2

Matrix Representation

0	-0.5	-0.015265763
-0.505547115	-0.252773558	-0.252773558
0	0	-0.835135083

	a	b	c
	0.505547115	0.560262859	0.872684434
	81.58784777	73.16296173	63.18125235
	alpha	beta	gamma

Normalized Niggli Matrix

1	1.228175397	2.979827926
0.279865187	0.5	0.5

Daughter 15e
Ref. Lattice 70a

	|G|	Z	|G|/Z
	4	2	2
	8	2	4
		1	2
		(size)	(index)

Reduced Cell

Character	27 (mC)	… but close to 26 (oF)
Type	I	
b.b≥a.a	True	|b.c|≤b.b/2 True
c.c≥b.b	True	|a.c|≤a.a/2 True
2|D+E+F| ≤ A+B	N/A	|a.b|≤a.a/2 True

Transformation to Conventional Cell

1	-1	-1	0
0	2	0	0
0	0	2	0
0	0	0	1

Det= 4

Overall Transformation

0	-1	0	0.75
-1	0	0.5	0
0	0	-0.5	0.25
0	0	0	1

Det= 0.5

2 nearest neighbors
6 neighbors within 2% of nearest
10 neighbors within 13% of nearest
next neighbor 24% farther than nearest
sphere packing

Center of Mass Coordinates

		e	2						
0,y,1/4	0	0.377	0.25	1	x,1/4,1/4	0.123	0.25	0.25	1
0,1-y,3/4	0	0.623	0.75	1	1-x,3/4,3/4	-0.123	0.75	-0.25	1
1/2,1/2+y,1	0.5	0.877	0.25	1		0.123	-0.75	0.25	1
1/2,1/2-y,3/4	0.5	0.123	0.75	1		0.877	-0.25	-0.25	1

y= 0.377

Z'= 2

Order Parameter = GM3+

Very distorted diamond cubic.
Close to particular distortion w/ 10 nearest neighbors.

15e C2/n

48 TFMETH02

a= 8.40982
b= 4.30221 b/a= 0.5115698
c= 8.35062 c/a= 0.9929606
alpha= 90 alpha= 90
beta= 119.5881 beta= 119.5881
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.490285
0	0.5115698	0
0	0	0.8634761

	a	b	c
	1	0.5115698	0.9929606
	90	119.5881	90
	alpha	beta	gamma

Transformation to Reduced Cell

0	-0.5	-0.5	0.5
-1	-0.5	-0.5	0.5
0	0	-1	1
0	0	0	1

Det= 0.5

Inverse Transformation

1	-1	0	0
-2	0	1	0
0	0	-1	1
0	0	0	1

Det= 2

Matrix Representation

0	-0.5	-0.009714511
-0.511569808	-0.255784904	-0.255784904
0	0	-0.863476064

	a	b	c
	0.511569808	0.561627917	0.900617123
	82.01283561	73.50027726	62.90708582
	alpha	beta	gamma

Normalized Niggli Matrix

1	1.20527893	3.099349763
0.268560135	0.5	0.5

See #47 above.

6 neighbors within 6% of nearest
10 neighbors within 12% of nearest
next neighbor 20% farther than nearest
sphere packing

Center of Mass Coordinates

See above.

		e	2						
1/4,y,1/4	0.25	0.32562	0.25	1	-x,3/4,3/4	-0.07562	-0.25	0.75	1
1/4,1/2-y,3/4	0.25	0.17438	0.75	1	x,1/4,1/4	0.07562	0.25	0.25	1
3/4,1/2+y,1	0.75	0.82562	0.25	1		-0.07562	-1.25	0.75	1
3/4,1-y,3/4	0.75	0.67438	0.75	1		0.07562	-0.75	0.25	1

y= 0.32562

15e C2/c

49 REKYUB

a= 19.8721
b= 9.49968 b/a= 0.4780411
c= 19.7822 c/a= 0.9954761
alpha= 90 alpha= 90
beta= 123.4156 beta= 123.4156
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.548217
0	0.4780411	0
0	0	0.8309218

	a	b	c
	1	0.4780411	0.9954761
	90	123.4156	90
	alpha	beta	gamma

Transformation to Reduced Cell

0	0	0.5	0
-1	0	0.5	0.5
0	-0.5	0.5	0.25
0	0	0	1

Det= 0.25

Inverse Transformation

1	-1	0	0.5
2	0	-2	0.5
2	0	0	0
0	0	0	1

Det= 4

Matrix Representation

0	0.27410833	0.22589167
-0.478041073	0	0.239020536
0	-0.415460918	0.415460918

	a	b	c
	0.478041073	0.497738035	0.529873228
	114.8151994	116.8136414	90
	alpha	beta	gamma

Normalized Niggli Matrix

1	1.084104714	1.228608542
-0.484366374	-0.5	6.37814E-17

Daughter 15e
Ref. Lattice FCC

	|G|	Z	|G|/Z
	4	2	2
	48	1	48
		2	24
		(size)	(index)

Reduced Cell

Character	37 (mC)	… but close to singularity: 1 (cF)
Type	II	
b.b≥a.a	True	|b.c|≤b.b/2 True
c.c≥b.b	True	|a.c|≤a.a/2 True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2 True

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

-0.5	-0.5	1	0
1	0	0	0
-0.5	0.5	1	-0.5
0	0	0	1

Det= 1

12 neighbors within 16% of nearest
next neighbor 41% farther than nearest
sphere packing

Center of Mass Coordinates

		e	2						
0,y,1/4	0	0.5238033	0.25	1	0,0,0	-0.023803333	0	0	1
0,1-y,3/4	0	0.4761967	0.75	1		0.023803333	-1	0	1
1/2,1/2+y,1	0.5	0.0238033	0.25	1		0.976196667	1	1	1
1/2,1/2-y,3/4	0.5	0.9761967	0.75	1		0.023803333	0	1	1

y= 0.5238033

error	-0.023803333	0	0

Z'= 1

Order Parameter = Coupled

12i C2/m

50 MECKOU

a= 15.7928
b= 11.5117 b/a= 0.7289208
c= 18.4079 c/a= 1.1655881
alpha= 90 alpha= 90
beta= 109.736 beta= 109.736
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.393604
0	0.7289208	0
0	0	1.0971198

	a	b	c
	1	0.7289208	1.1655881
	90	109.736	90
	alpha	beta	gamma

Transformation to Reduced Cell

0.5	0.5	0.5	0.25
-0.5	0.5	0	0
0	0	0.5	0.25
0	0	0	1

Det= 0.25

Inverse Transformation

1	-1	-1	0
1	1	-1	0
0	0	2	-0.5
0	0	0	1

Det= 4

Matrix Representation

0.5	0.5	0.303198177
-0.364460387	0.364460387	0
0	0	0.548559893

	a	b	c
	0.618733686	0.618733686	0.626775152
	66.98862618	66.98862618	72.17816954
	alpha	beta	gamma

Normalized Niggli Matrix

1	1	1.026162217
0.395994422	0.395994422	0.306058057

Daughter 12i
Ref. Lattice FCC

	|G|	Z	|G|/Z
	4	2	2
	48	1	48
		2	24
		(size)	(index)

Reduced Cell

Character	14 (mC)	along rhom path from FCC to BCC
Type	I	
b.b≥a.a	True	|b.c|≤b.b/2 True
c.c≥b.b	True	|a.c|≤a.a/2 True
2|D+E+F| ≤ A+B	N/A	|a.b|≤a.a/2 True

Transformation to Conventional Cell

-1	1	1	0
1	-1	1	0
1	1	-1	0
0	0	0	1

Det= 4

Overall Transformation

0.5	0.5	0.5	-0.25
0.5	-0.5	0.5	-0.25
1	0	-1	0
0	0	0	1

Det= 1

12 neighbors within 19% of nearest
next neighbor 40% farther than nearest

Center of Mass Coordinates

sphere packing

	i	m			
x,0,z	0.2535	0	0.2411	1	
1-x,1,1-z	0.7465	1	0.7589	1	
1/2+x,1/2,z	0.7535	0.5	0.2411	1	
1/2-x,1/2,1-	0.2465	0.5	0.7589	1	
x=	0.2535				
z=	0.2411				

0,0,0

0.0124	0.0124	-0.0178	1	Z'= 1
-1.0124	0.9876	1.0178	1	
0.0124	1.0124	-0.0178	1	
-1.0124	-0.0124	1.0178	1	

error 0.0124 0.0124 -0.0178

Order Parameter = Coupled

11e P_21/m

51 MECKIO

a=	9.5283		
b=	15.3492	b/a=	1.6109065
c=	10.7393	c/a=	1.1270951
alpha=	90	alpha=	90
beta=	104.954	beta=	104.954
gamma=	90	gamma=	90

2 nearest neighbors
2 next neighbors not coplanar

Matrix Representation

1	0	-0.29084	
0	1.6109065	0	
0	0	1.0889241	

a	b	c
1	1.6109065	1.1270951
90	104.954	90
alpha	beta	gamma

Transformation to Rod Coordinates

0	0.29084	1	0.20498
1	0	0	0.25
0	1	0	0.219284
0	0	0	1

Det= 1

Inverse Transformation

0	1	0	-0.25
0	0	1	-0.219284
1	0	-0.29084	-0.141203
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.581364682	0.581364682	0	0
-0.860045365	0.860045365	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.860045365	-0.581364682	0	0
0.860045365	0.581364682	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0	0	1	
0.93652412	0.93652412	0	
-0.936524 12	0.93652412	0	

a	b	c
1.324445112	1.324445112	1
89.99999743	90.00000257	90
alpha	beta	gamma

p-42m (#37)
2nd setting

Daughter	11e	4	2	2
Rod	37a	8	1	8
			2	4
			(size)	(index)

Hexagonal packing of p-42m rods

Center of Mass Coordinates

	e	m		
i	x,1/4,z	0.2049796	0.25	0.2192841	1
	1-x,3/4,1-z	0.7950204	0.75	0.7807159	1
	x=	0.2049796			
	z=	0.2192841			

Molecular 3-fold axes

	f	1			
i	x,y,z	0.0917	0.1478	0.2244	1
i	x,1/2-y,z	0.0917	0.3522	0.2244	1
	e	m			
i	x,1/4,z	0.2782	0.25	0.0701	1
i		0.3715	0.25	0.3735	1

rod axis:

1	0	0

rod origin:

0.20498	0.25	0.219284

Transformation to orthogonal axes:

0.29084

rotation angle:

45 degrees

Rescaling parameter:

0.822173817

a m2m

0,0,0

0	0	0	1	Z'= 1
0.103626103	0.756419262	0.426754	1	

f m

-x,-x,z	-0.09087082	-0.084922453	-0.114767	1
x,x,z	0.084922453	0.09087082	-0.114767	1
x,-x,-z	0.086730387	-0.086730387	0.116609	1
-x,x,-z	-0.089655658	0.089655658	0.121668	1
error	-0.003122377	0.002825991	0.002186	

x= 0.088044829
z= -0.116953091

14e P_21/c

52 CAMPOV

a=	10.3894		
b=	14.6835	b/a=	1.4133155
c=	16.9885	c/a=	1.6351762
alpha=	90	alpha=	90
beta=	91.61	beta=	91.61
gamma=	90	gamma=	90

3 neighbors within 4% of nearest
next neighbor 26% farther than nearest

Matrix Representation

1	0	-0.045942	
0	1.4133155	0	
0	0	1.6345307	

a	b	c
1	1.4133155	1.6351762
90	91.61	90
alpha	beta	gamma

Transformation to Planar Coordinates

0	0.045942	1	0
1	0	0	0
0	1	0	0
0	0	0	1

Det= 1

Inverse Transformation

0	1	0	0
0	0	1	0
1	0	-0.045942	0
0	0	0	1

Det= 1

Rotation about plane normal and rescaling:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

8.65761E-17	0	1	
1.413315495	1.02981E-16	0	
0	1.634530713	0	

a	b	c
1.413315495	1.634530713	1
90	90	90
alpha	beta	gamma

p2gg (#8) in projection
2_1/c when accounting for 3rd dimension

Daughter	14e	4	4	1
Plane	2_1/c	4	4	1
			1	1
			(size)	(index)

planar packing

Center of Mass Coordinates

	e	1		
x,y,z	0.1712083	0.0255667	0.2124792	1
1-x,1/2+y,1	0.8287917	0.5255667	0.2875208	1
1-x,1-y,1-z	0.8287917	0.9744333	0.7875208	1
x,1/2-y,1/2·	0.1712083	0.4744333	0.7124792	1
x=	0.1712083			
y=	0.0255667			
z=	0.2124792			

plane normal:

1	0	0

plane origin:

0	0	0

Transformation to orthogonal axes:

0.045942

rotation angle:

0 degrees

x,y,z	0.025566667	0.212479167	0.161447	1	Z'= 4
1/2+x,1/2-y,-z	0.525566667	0.287520833	0.815582	1	
-x,-y,-z	0.974433333	0.787520833	0.792611	1	
1/2-x,1/2+y,z	0.474433333	0.712479167	0.138476	1	
x=	0.025566667				
y=	0.212479167				
z=	0.161446598				

error= 0 0 0

14e P_21/c

53 VAVYAS

a=	9.6783		
b=	14.3654	b/a=	1.4842896
c=	17.0195	c/a=	1.7585216
alpha=	90	alpha=	90
beta=	92.242	beta=	92.242
gamma=	90	gamma=	90

3 neighbors within 4% of nearest
next neighbor 27% farther than nearest
planar packing

Matrix Representation

1	0	-0.068794
0	1.4842896	0
0	0	1.7571755

a	b	c
1	1.4842896	1.7585216
90	92.242	90
alpha	beta	gamma

See #52 above.

See above.

Center of Mass Coordinates

	e	1		
x,y,z	0.3443616	0.5277806	0.2914611	1
1-x,1/2+y,1	0.6556384	0.0277806	0.2085389	1
1-x,1-y,1-z	0.6556384	0.4722194	0.7085389	1
x,1/2-y,1/2·	0.3443616	0.9722194	0.7914611	1
x=	0.3443616			
y=	0.5277806			
z=	0.2914611			

14e P_21/c

54 CARBTC

a=	9.07912		
b=	5.7643	b/a=	0.6348963
c=	9.2014	c/a=	1.0134683
alpha=	90	alpha=	90
beta=	104.295	beta=	104.295
gamma=	90	gamma=	90

1 nearest neighbor
3 neighbors within 6% of nearest
next neighbor 11% farther than nearest

Matrix Representation

1	0	-0.25024	
0	0.6348963	0	
0	0	0.9820885	

a	b	c
1	0.6348963	1.0134683
90	104.295	90
alpha	beta	gamma

Transformation to Reduced Cell

0	-1	0	1
-1	0	0	1
0	0	-1	1
0	0	0	1

Det= 1

Inverse Transformation

0	-1	0	1
-1	0	0	1
0	0	-1	1
0	0	0	1

Det= 1

Matrix Representation

0	-1	0.250239959
-0.634896334	0	0
0	0	-0.982088534

a	b	c
0.634896334	1	1.013468266
104.295	90	90
alpha	beta	gamma

Normalized Niggli Matrix

1	2.480814901	2.548089455
-0.620799018	9.77836E-17	9.64841E-17

Reduced Cell

Character	35 (mP)	… but close to 23 (oC)
Type	II	
b.b≥a.a	True	|b.c|≤b.b/2 True
c.c≥b.b	True	|a.c|≤a.a/2 True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2 True

Center of Mass Coordinates

	e	1			
i	x,y,z	0.248	0.067	0.157	1
ii	1-x,1/2+y,1	0.752	0.567	0.343	1
i	1-x,1-y,1-z	0.752	0.933	0.843	1
ii	x,1/2-y,1/2·	0.248	0.433	0.657	1
x=		0.248			
y=		0.067			
z=		0.157			

0.933	0.752	0.843	1	Z'= 4
0.433	0.248	0.657	1	
0.067	0.248	0.157	1	
0.567	0.752	0.343	1	

dimers:

Transformation to Reduced Cell

0	0	-1	0

Matrix Representation

-0.125119979	-0.125119979	-1

	|G|	Z	|G|/Z
Daughter	14e	4	4	1
Plane	2_1/c	4	4	1
		1	1	

Transformation to Conventional Cell

1	-1	-1	0

Dimer Coordinates (a), -1 WP symmetry ensures Cs dimer symmetry
4 nearest neighbors, all coplanar (bc-plane)
next neighbor 6% farther, also co-planar
next neighbor 67% farther than nearest
packing of dimers

-0.5	0.5	0	0
0.5	0.5	0	0
0	0	0	1

Det= 0.5

-0.317448167	0.317448167	0
0.491044267	0.491044267	0

a	b	c
0.597957206	0.597957206	1
77.92184748	77.92184748	64.13091485
alpha	beta	gamma

Daughter	14e	4	4	1
Cs Dimers	12a	4	1	4
Ref. Lattice	166a	12	1	12
			1	3
			(size)	(index)

0	1	-1	0
0	0	3	0
0	0	0	1

Det= 3

Inverse Transformation

0	-1	1	0
0	1	1	0
-1	0	0	0
0	0	0	1

Det= 2

Normalized Niggli Matrix

1	1	2.796789577
0.349934254	0.349934254	0.436316354

Reduced Cell

Character	10 (mC)	… but close to 9 (hR)	
Type	I		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	N/A	|a.b|≤a.a/2	True

Overall Transformation

-0.666667	0	2	0
-0.333333	1	1	0
-0.333333	0	0	0
0	0	0	1

Det= 0.666667

Dimer Center of Mass Coordinates

	a -1													
i	0,0,0	0	0	0	1	0,0,0	0	0	0	1	Z' = 1			Order Parameter = F2+
ii	0,1/2,1/2	0	0.5	0.5	1		0	1	0	1				

14e P_21/c
55 QUGBOJ

a=	16.1133		
b=	9.5502	b/a=	0.5926905
c=	17.0133	c/a=	1.0558545
alpha=	90	alpha=	90
beta=	104.893	beta=	104.893
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.27137
0	0.5926905	0
0	0	1.0203857

a	b	c
1	0.5926905	1.0558545
90	104.893	90
alpha	beta	gamma

Transformation to Rod Coordinates

0	1	0	0.25
-1	0	0	0.75
0	0.243414	1	0
0	0	0	1

Det= 1

Inverse Transformation

0	-1	0	0.75
1	0	0	-0.25
-0.243414	0	1	0.060854
0	0	0	1

Det= 1

Rotation about rod and rescaling:

1.276927253	0	0	0
0	0.783129969	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.783129969	0	0	0
0	1.276927253	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

-4.6361E-17	0.731400026	0
-1	0	8.13E-17
0	0.194511051	1.020386

a	b	c
0.756822665	0.756822665	1.055854
90.00027569	90	90
alpha	beta	gamma

pc11 (#5)

Daughter	14e	4	4	1
Rod	5a	2	2	1
			2	1
			(size)	(index)

4 neighbors within 2% of nearest
next neighbor 10% farther than nearest

Hexagonal packing of pc11 rods

Center of Mass Coordinates

	e 1				
x,y,z	0.2324831	0.8707496	0.4302323	1	
1-x,1/2+y,1	0.7675169	0.3707496	0.0697677	1	
1-x,1-y,1-z	0.7675169	0.1292504	0.5697677	1	
x,1/2-y,1/2-	0.2324831	0.6292504	0.9302323	1	
x=	0.2324831				
y=	0.8707496				
z=	0.4302323				

rod axis:

0	0	1

rod origin:

0.25	0.75	0

Transformation to orthogonal axes:
0.243414

rotation angle:
0

Rescaling parameter:
1.276927253 1

a 1

x,y,z	-0.094562635	-0.0223678	0.434496	1
	0.29700235	0.660831427	-0.056203	1
	0.486127619	0.660831427	0.443797	1
-x,y,z+1/2	0.094562635	-0.0223678	0.934496	1

Z' = 2

14e P_21/n
56 DOCNIS

a=	8.4595		
b=	12.2587	b/a=	1.4491046
c=	13.1488	c/a=	1.5543235
alpha=	90	alpha=	90
beta=	93.285	beta=	93.285
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.089067
0	1.4491046	0
0	0	1.5517696

a	b	c
1	1.4491046	1.5543235
90	93.285	90
alpha	beta	gamma

Transformation to Rod Coordinates

0	1	0	0.5
0	0	1	0
1	0.036867	0	0.5
0	0	0	1

Det= 1

Inverse Transformation

-0.036867	0	1	-0.481567
1	0	0	-0.5
0	1	0	0
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.801442168	0	0	0
0	1.247750667	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.247750667	0	0	0
0	0.801442168	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

-0.071381948	1.243653563	0
0	0	1.449105
1.24365356	0.07138189	0

a	b	c
1.245700429	1.245700429	1.449105
90	90	90
alpha	beta	gamma

p-1 (#2)

Daughter	14e	4	4	1
Rod	2c	2	2	1
			2	1
			(size)	(index)

2 neighbors within 3% of nearest
next neighbor 10% farther than nearest

Hexagonal packing of p-1 rods

Center of Mass Coordinates

	e 1				
i	x,y,z	0.3257927	0.254875	0.4281235	1
ii	1-x,1-y,1-z	0.6742073	0.745125	0.5718765	1
	1/2-x,1/2+y	0.1742073	0.754875	0.0718765	1
	1/2+x,1/2-y	0.8257927	0.245125	0.9281235	1
	x=	0.3257927			
	y=	0.254875			
	z=	0.4281235			

rod axis:

0	1	0

rod origin:

0.5	0	0.5

Transformation to orthogonal axes:
0.036867

rotation angle:
0

Rescaling parameter:
0.801442168

c 1

x,y,z	-0.081670409	-0.139617052	0.254875	1
-x,-y,-z	0.081670409	0.139617052	0.745125	1

c 1

x,y,z	0.045712545	-0.057303115	0.3111	1
-x,-y,-z	-0.045712545	0.057303115	0.6889	1

Z' = 1

Molecular 3-fold axes

	e 1				
i	x,y,z	0.4285	0.3111	0.534	1
ii	x,y,z	0.5715	0.6889	0.466	1
	x=	0.4285			
	y=	0.3111			
	z=	0.534			

14e P_21/c
57 TMSIAD

a=	8.8592		
b=	9.8442	b/a=	1.1111839
c=	18.3163	c/a=	2.0674892
alpha=	90	alpha=	90
beta=	91.073	beta=	91.073
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.038716
0	1.1111839	0
0	0	2.0671266

a	b	c
1	1.1111839	2.0674892
90	91.073	90
alpha	beta	gamma

Transformation to Rod Coordinates

0	1	0	0
0	0	1	0
1	0.009057	0	0
0	0	0	1

Det= 1

Inverse Transformation

-0.009057	0	1	0
1	0	0	0
0	1	0	0
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.521466571	0.46007203	0	0
-0.95136076	1.078315571	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1.078315571	-0.46007203	0	0
0.95136076	0.521466571	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

-0.971216454	1.060125106	0
0	0	1.111184
1.060125296	0.97121623	0

a	b	c
1.437750689	1.437750398	1.111184
90	90	90
alpha	beta	gamma

p-1 (#2)

Daughter	14e	4	4	2
Rod	2c	2	1	2
			2	1
			(size)	(index)

2 neighbors within 4% of nearest
next neighbor 24% farther than nearest

Square packing of p-1 rods

Center of Mass Coordinates

	e 1				
i	x,y,z	-0.169642	0.2582289	0.0914053	1
ii	1-x,1-y,1-z	0.1696421	0.7417711	-0.091405	1
	1-x,1/2+y,1	0.1696421	0.7582289	0.4085947	1
	x,1/2-y,1/2-	-0.169642	0.2417711	0.5914053	1
	x=	-0.169642			
	y=	0.2582289			
	z=	0.0914053			

rod axis:

0	1	0

rod origin:

0	0	0

Transformation to orthogonal axes:
0.009057

rotation angle:
41.42085259

Rescaling parameter:
0.695408986

c 1

x,y,z	0.178268157	-4.15243E-05	0.258229	1
-x,-y,-z	-0.178268157	4.15243E-05	0.741771	1

c 1

x,y,z	0.240208951	-0.002109429	0.4381	1
-x,-y,-z	-0.240208951	0.002109429	0.5619	1

Z' = 1

Molecular 3-fold axes

	e 1				
i	x,y,z	-0.2308	0.4381	0.1222	1
ii	x,y,z	0.2308	0.5619	-0.1222	1
	x=	-0.2308			
	y=	0.4381			
	z=	0.1222			

14e P_21/n
58 MECKUA

a=	16.7235		
b=	11.1082	b/a=	0.664227
c=	19.1055	c/a=	1.1424343
alpha=	90	alpha=	90
beta=	112.703	beta=	112.703
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.440927
0	0.664227	0
0	0	1.0539161

a	b	c
1	0.664227	1.1424343
90	112.703	90
alpha	beta	gamma

Transformation to Reduced Cell

-0.5	-0.5	-0.5	0
0	-0.5	0.5	0.25
-0.5	0	0	0.25
0	0	0	1

Det= 0.25

Inverse Transformation

0	0	-2	0.5

Matrix Representation

-0.279536259	-0.5	-0.5
0	-0.332113493	0.332113493
-0.526958035	0	0

a	b	c
0.596510931	0.600249425	0.600249425
67.1863708	67.02350771	67.02350771
alpha	beta	gamma

Reduced Cell

Character	20 (mC)	…but close to 1 (cF)	

Daughter	14e	|G|	Z	|G|/Z
Ref. Lattice	FCC	4	4	1
		48	1	48
			4	48
			(size)	(index)

Transformation to Conventional Cell

-1	1	1	0
1	-1	1	0
1	1	-1	0
0	0	0	1

Det= 4

Overall Transformation

12 neighbors within 14% of nearest
next neighbor 45% farther than nearest
sphere packing

-1	-1	1	0	
-1	1	1	-0.5	
0	0	0	1	

Det= 4

Normalized Niggli Matrix

1	1.012573816	1.012573816
0.39261017	0.392799874	0.392799874

Type I
b.b≥a.a True
c.c≥b.b True
2|D+E+F| ≤ A+B N/A

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

-1	0	1	-0.25
-0.5	0.5	-0.5	0
-0.5	-0.5	-0.5	0.25
0	0	0	1

Det= 1

Center of Mass Coordinates

e 1

x,y,z	0.0013148	0.2747839	0.2493133	1
1-x,1-y,1-z	0.9986852	0.7252161	0.7506867	1
1/2-x,1/2+y	0.4986852	0.7747839	0.2506867	1
1/2+x,1/2-y	0.5013148	0.2252161	0.7493133	1

x= 0.0013148
y= 0.2747839
z= 0.2493133

0,0,0

0.001373469	-0.026785469	0.022782313	1
-1.001373469	-0.973214531	-0.022782313	1
-0.001373469	-1.022782313	0.026785469	1
-0.998626531	0.022782313	-0.026785469	1

error 0.001373469 -0.026785469 0.022782313

Z'= 1

Along Rhom. Path from FCC to BCC

Order Parameter = Coupled

14e P_21/c
59 TOHSUE

a= 10.4005
b= 10.5225 b/a= 1.0117302
c= 28.7446 c/a= 2.763771
alpha= 90 alpha= 90
beta= 90 beta= 90
gamma= 90 gamma= 90

Matrix Representation

1	0	0
0	1.0117302	0
0	0	2.763771

a	b	c
1	1.0117302	2.763771
90	90	90
alpha	beta	gamma

Transformation to Reduced Cell

-0.5	-0.5	0.5	0.25
-0.5	0.5	-0.5	0.75
0.25	-0.25	-0.25	0.125
0	0	0	1

Det= 0.25

Inverse Transformation

-1	-1	0	1
-1	0	-2	0.5
0	-1	-2	1
0	0	0	1

Det= 4

Matrix Representation

-0.5	-0.5	0.5
-0.505865103	0.505865103	-0.505865103
0.690942743	-0.690942743	-0.690942743

a	b	c
0.991615539	0.991615539	0.991615539
91.66075478	118.653373	119.4398054
alpha	beta	gamma

Reduced Cell
Character 8 (oI) … but close to singularity: 1 (cF)
Type II
b.b≥a.a True
c.c≥b.b True
2|D+E+F| ≤ A+B Equal

|b.c|≤b.b/2 True
|a.c|≤a.a/2 True
|a.b|≤a.a/2 True

Daughter 14e
Ref. Lattice FCC

|G|	Z	|G|/Z
	4	4	1
	48	1	48
		4	48
		(size)	(index)

Transformation to Conventional Cell

0	0	2	0
1	1	1	0
-1	1	1	0
0	0	0	1

Det= 4

Overall Transformation

-0.5	0.5	0	-0.25
0	0	-2	0.25
-0.5	-0.5	0	0.5
0	0	0	1

Det= 1

12 neighbors within 3% of nearest
next neighbor 40% farther than nearest
sphere packing

Normalized Niggli Matrix

1	1	1
-0.02898158	-0.479509521	-0.491508898

Center of Mass Coordinates

e 1

x,y,z	0.2504837	0.7448743	0.1256666	1
1-x,1/2+y,1	0.7495163	0.2448743	0.3743334	1
1-x,1-y,1-z	0.7495163	0.2551257	0.8743334	1
x,1/2-y,1/2-	0.2504837	0.7551257	0.6256666	1

x= 0.2504837
y= 0.7448743
z= 0.1256666

0,0,0

0.004641935	-0.001816854	0.003792581	1
0.005609435	-0.998183146	0.00645879	1
-0.004641935	-1.998183146	-1.003792581	1
-0.005609435	-1.001816854	-1.00645879	1

error 0.004641935 -0.001816854 0.003792581

Z'= 1

Order Parameter = Coupled

14ee P_21/n
60 CANFIG

a= 18.2286
b= 16.7496 b/a= 0.9188638
c= 8.7652 c/a= 0.4808488
alpha= 90 alpha= 90
beta= 90.694 beta= 90.694
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.005824
0	0.9188638	0
0	0	0.4808135

a	b	c
1	0.9188638	0.4808488
90	90.694	90
alpha	beta	gamma

Transformation to Planar Coordinates

0.005824	0	1	0.25
0	1	0	0
1	0	0	0.25
0	0	0	1

Det= -1

Inverse Transformation

0	0	1	-0.25
0	1	0	0
1	0	-0.005824	-0.248544
0	0	0	1

Det= -1

Rotation about plane normal and rescaling:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

-5.7798E-08	5.62872E-17	1
2.98123E-17	0.918863764	0
0.480813503	0	0

a	b	c
0.480813503	0.918863764	1
90	90.00000689	90
alpha	beta	gamma

pg (##) in projection
distorted p6mm (#17) - puckered honeycomb
2_1 when accounting for 3rd dimension

Daughter 14ee
Plane 2_1

|G|	Z	|G|/Z
4	8	0.5
2	4	0.5
	2	1
	(size)	(index)

e: 3 neighbors within 6% of nearest
next neighbor 28% farther than nearest

e: 3 neighbors within 6% of nearest
next neighbor 30% farther than ne
planar

Center of Mass Coordinates

e 1

x,y,z	0.2987978	0.5073711	-0.02555	1
1-x,1-y,1-z	0.7012022	0.4926289	1.02555	1
1/2-x,1/2+y	0.2012022	0.0073711	0.52555	1
1/2+x,1/2-y	0.7987978	0.9926289	0.47445	1

x= 0.2987978
y= 0.5073711
z= -0.02555

plane normal:

1	0	0

plane origin:

0.25	0	0.25

Transformation to orthogonal axes:

0.005824		

rotation angle:

0 degrees

-x,1/2+y,-z	-0.27555	0.507371111	0.050403	1
	0.77555	0.492628889	0.446685	1
x,y,z	0.27555	0.007371111	-0.050403	1
	0.22445	0.992628889	0.547491	1

x= 0.27555
y= 0.007371111
z= 0.050402614

Z'= 4

e 1

x,y,z	0.37146	0.17384	0.0347222	1
1-x,1-y,1-z	0.62854	0.82616	0.9652778	1
1/2-x,1/2+y	0.12854	0.67384	0.4652778	1
1/2+x,1/2-y	0.87146	0.32616	0.5347222	1

x= 0.37146
y= 0.17384
z= 0.0347222

x,y,z	-0.215277778	0.17384	0.122714	1
	0.715277778	0.82616	0.374374	1
-x,1/2+y,-z	0.215277778	0.67384	-0.122714	1
	0.284722222	0.32616	0.619802	1

x= -0.215277778
y= 0.17384
z= 0.122713804

14ee P_21/a
61 MXSNOX

a= 18.3874
b= 18.5194 b/a= 1.0071788
c= 10.5433 c/a= 0.5733981
alpha= 90 alpha= 90
beta= 104.742 beta= 104.742
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.145911
0	1.0071788	0
0	0	0.5545227

a	b	c
1	1.0071788	0.5733981
90	104.742	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	0	0	0.071518
0	1	0	0.274913
0.443769	0	1	0.158782
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	-0.071518
0	1	0	-0.274913
-0.443769	0	1	-0.127045
0	0	0	1

Det= 1

Rotation about rod and rescaling:

0.809124867	0.62191573	0	0
-0.597156301	0.776912352	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.776912352	-0.62191573	0	0
0.597156301	0.809124867	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

0.756733494	0.581646273	0
-1	1	4.41E-17
0.199109283	0.153040897	0.554523

a	b	c
0.986926538	0.986926538	0.573398
90.00039009	90.00050751	90
alpha	beta	gamma

p11c (#5)
… but nearly pmcm (#22)

Daughter 14ee
Rod 22b

|G|	Z	|G|/Z
4	8	0.5
8	2	4
	4	8
	(size)	(index)

Center of Mass Coordinates

e: 1 nearest neighbor
next neighbor less than 1% farther
next neighbor 4% farther than nearest

e 1

x,y,z	0.9989317	0.8207	0.1219222	1
1-x,1-y,1-z	0.0010683	0.1793	0.8780778	1
1/2-x,1/2+y	0.5010683	0.3207	0.8780778	1
1/2+x,1/2-y	0.4989317	0.6793	0.1219222	1

x= 0.9989317
y= 0.8207
z= 0.1219222

rod axis:

0	0	1

rod origin:

0.071518	0.274913	0.158782

Transformation to orthogonal axes:

0.443769		

rotation angle:

37.546875

Rescaling parameter:

1.020520566

b m2m

0,-y,3/4	0.381085562	0.995420431	-0.448417	1
	0.004729961	-0.119432636	0.750559	1
	0.305247253	0.293555771	0.528675	1
	0.08056827	0.582432024	-0.226533	1

Z'= 2

e: 1 nearest neighbor
next neighbor less than 1% farther
next neighbor 4% farther than nearest

e 1

x,y,z	0.8550967	0.6405294	0.5592111	1
1-x,1-y,1-z	0.1449033	0.3594706	0.4407889	1
1/2-x,1/2+y	0.6449033	0.1405294	0.4407889	1
1/2+x,1/2-y	0.3550967	0.8594706	0.5592111	1

x= 0.8550967
y= 0.6405294
z= 0.5592111

b m2m

0,y,1/4	0.381389276	0.763747978	0.052701	1
	0.004426247	0.112239818	0.249441	1
	0.529045344	0.233667271	0.027556	1
	-0.143229821	0.642320525	0.274586	1

y= 0.115836227

error= 0.004426247 -0.003596409 -0.000559

13efg P_2/c
62 RIMNAC

a= 18.3422
b= 9.51838 b/a= 0.5189334
c= 33.8124 c/a= 1.8434212
alpha= 90 alpha= 90
beta= 94.3008 beta= 94.3008
gamma= 90 gamma= 90

Matrix Representation

1	0	-0.138243
0	0.5189334	0
0	0	1.8382303

a	b	c
1	0.5189334	1.8434212
90	94.3008	90
alpha	beta	gamma

Transformation to Rod Coordinates

1	-0.138243	0	0
0	0	1	0.481138
0	-1	0	0.25
0	0	0	1

Det= 1

Inverse Transformation

1	0	-0.138243	0.034561
0	0	-1	0.25
0	1	0	-0.481138

Rotation about rod and rescaling:

1.354553635	-0.058435591	0	0
0.031789048	0.736879192	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.736879192	0.058435591	0	0
-0.031789048	1.354553635	0	0
0	0	1	0

Matrix Representation

1.354553635	-0.058435588	0
-3.85892E-18	-8.94451E-17	1
-0.058435591	-1.354553635	0

a	b	c
1.355813508	1.355813507	0.518933
90	90	90
alpha	beta	gamma

p-42m (#37)

Daughter 13efg
Rod 37a

|G|	Z	|G|/Z
4	8	0.5
8	1	8
	8	16
	(size)	(index)

0	0	0	1		0	0	0	1		2nd setting
		Det= 1					Det= 1			

Center of Mass Coordinates

e: 2 nearest neighbors	e 2	Unique axis b, Cell Choice 1			
4 neighbors within 2% of nearest	0,y,1/4	0	0.4811384	0.25	1
next neighbor 5% farther than nearest	0,1-y,3/4	0	0.5188616	0.75	1
	y=	0.4811384			
f: 2 nearest neighbors	f 2	Unique axis b, Cell Choice 1			
4 neighbors within 2% of nearest	1/2,y,1/4	0.5	0.8131861	0.25	1
next neighbor 3% farther than nearest	1/2,1-y,3/4	0.5	0.1868139	0.75	1
	y=	0.8131861			
g: 1 nearest neighbor	g 1	Unique axis b, Cell Choice 1			
3 neighbors within 1% of nearest	x,y,z	0.2557004	0.1578597	0.0006353	1
next neighbor 4% farther than nearest	1-x,y,1/2-z	0.7442996	0.1578597	0.4993647	1
	1-x,1-y,1-z	0.7442996	0.8421403	0.9993647	1
Hexagonal packing of p-42m rods	x,1-y,1/2+z	0.2557004	0.8421403	0.5006353	1
with 3 independent orientations	x=	0.2557004			
	y=	0.1578597			
	z=	0.0006353			

rod axis:
0 1 0

rod origin:

0	0.481138	0.25	(e)
0.5	0.813186	0.25	(f)
0.25	0.15786	0	(g)

Transformation to orthogonal axes:
-0.138243

rotation angle:
-2.470214495 degrees

Rescaling parameter:
1.355813508

a	-42m				
0,0,0	0	0	0	1	Z'= ?
f	..m				
x,-x,z	0.038779225	-0.038313953	0.099762	1	
-x,x,z	-0.038779225	0.038313953	0.099762	1	
-x,-x,-z	-0.038830444	-0.038222842	-0.102438	1	
x,x,-z	0.038830444	0.038222842	-0.102438	1	
x=	0.038536616				
z=	0.1011				
error=	0.000242609	0.000222663	-0.001338		
	-0.000242609	-0.000222663	-0.001338		
	-0.000293828	0.000313774	-0.001338		
	0.000293828	-0.000313774	-0.001338		

Molecular 3-fold axes
g 1

x,y,z	0.0585	0.5809	0.277	1
	-0.0585	0.5809	0.223	1
	-0.0463	0.3787	0.2794	1
	0.0463	0.3787	0.2206	1

15ffff C2/c
63 CTBROM

a=	21.434		
b=	12.122	b/a=	0.5655501
c=	21.024	c/a=	0.9808715
alpha=	90	alpha=	90
beta=	110.883	beta=	110.883
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.349642
0	0.5655501	0
0	0	0.9164383
a	b	c
1	0.5655501	0.9808715
90	110.883	90
alpha	beta	gamma

Transformation to Reduced Cell

0	0.5	0.5	0
-1	-0.5	-0.5	1
0	0	1	0
0	0	0	1

Det= 0.5

Inverse Transformation

-1	-1	0	1
2	0	-1	0
0	0	1	0
0	0	0	1

Det= 2

Matrix Representation

-3.46441E-17	1	0.150357756
-1	-0.28277503	-0.28277503
0	0	0.916438337
a	b	c
0.565550061	0.574422943	0.970787514
73.84672292	73.06514726	60.50966745
alpha	beta	gamma

Normalized Niggli Matrix

1	1.031624029	2.946498726
0.485046471	0.5	0.5

Daughter	15ffff
Ref. Lattice	FCC

|G|	Z	|G|/Z
4	16	0.25
48	1	48
	16	192
	(size)	(index)

Reduced Cell
Character 41 (mC) … but close to singularity: 1 (cF)

Type	I		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	N/A	|a.b|≤a.a/2	True

Transformation to Conventional Cell

1	1	-1	0
-1	1	-1	0
0	2	0	0
0	0	0	1

Det= 4

Overall Transformation

-1.5	-0.5	0.5	0.5
0	0	0.5	0
-0.5	0.5	1	-0.5
0	0	0	1

Det= 0.5

f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of neare Center of Mass Coordinates
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
sphere packing

0,0,0 Z'= 1 Order Parameter = Coupled

f 1									
x,y,z	0.0961	0.0316	0.3782	1	0.8723	-0.186	0.3782	1
1-x,y,1/2-z	0.9039	0.0316	0.1218	1	0.0645	1.686	0.1218	1
1-x,1-y,1-z	0.9039	0.9684	0.6218	1	-0.8723	1.186	0.6218	1
x,1-y,1/2+z	0.0961	0.9684	0.8782	1	-0.0645	-0.686	0.8782	1
1/2+x,1/2+	0.5961	0.5316	0.3782	1	-0.1277	0.814	0.3782	1
1/2-x,1/2+y	0.4039	0.5316	0.1218	1	0.0645	0.686	0.1218	1
1/2-x,1/2-y	0.4039	0.4684	0.6218	1	0.1277	0.186	0.6218	1
1/2+x,1/2-y	0.5961	0.4684	0.8782	1	-0.0645	0.314	0.8782	1
x=	0.0961							
y=	0.0316				0.5611	0.6383	0.1201	1
z=	0.3782				0.3195	0.8617	0.3799	1
f 1					-0.5611	0.3617	0.8799	1
x,y,z	0.3792	0.0597	0.1201	1	-0.3195	0.1383	0.6201	1
1-x,y,1/2-z	0.6208	0.0597	0.3799	1	-0.4389	1.6383	0.1201	1
1-x,1-y,1-z	0.6208	0.9403	0.8799	1	0.3195	-0.1383	0.3799	1
x,1-y,1/2+z	0.3792	0.9403	0.6201	1	0.4389	-0.6383	0.8799	1
1/2+x,1/2+	0.8792	0.5597	0.1201	1	-0.3195	1.1383	0.6201	1
1/2-x,1/2+y	0.1208	0.5597	0.3799	1				
1/2-x,1/2-y	0.1208	0.4403	0.8799	1	0.5581	0.129	0.1232	1
1/2+x,1/2-y	0.8792	0.4403	0.6201	1	-0.1897	1.371	0.3768	1
x=	0.3792				-0.5581	0.871	0.8768	1
y=	0.0597				0.1897	-0.371	0.6232	1
z=	0.1201				-0.4419	1.129	0.1232	1
f 1					-0.1897	0.371	0.3768	1
x,y,z	0.1261	0.3158	0.1232	1	0.4419	-0.129	0.8768	1
1-x,y,1/2-z	0.8739	0.3158	0.3768	1	0.1897	0.629	0.6232	1
1-x,1-y,1-z	0.8739	0.6842	0.8768	1				
x,1-y,1/2+z	0.1261	0.6842	0.6232	1	0.3641	0.3191	0.3713	1
1/2+x,1/2+	0.6261	0.8158	0.1232	1	0.0545	1.1809	0.1287	1
1/2-x,1/2+y	0.3739	0.8158	0.3768	1	-0.3641	0.6809	0.6287	1
1/2-x,1/2-y	0.3739	0.1842	0.8768	1	-0.0545	-0.1809	0.8713	1
1/2+x,1/2-y	0.6261	0.1842	0.6232	1	-0.6359	1.3191	0.3713	1
x=	0.1261				0.0545	0.1809	0.1287	1
y=	0.3158				0.6359	-0.3191	0.6287	1
z=	0.1232				-0.0545	0.8191	0.8713	1
f 1								
x,y,z	0.3452	0.2907	0.3713	1				
1-x,y,1/2-z	0.6548	0.2907	0.1287	1				
1-x,1-y,1-z	0.6548	0.7093	0.6287	1				
x,1-y,1/2+z	0.3452	0.7093	0.8713	1				
1/2+x,1/2+	0.8452	0.7907	0.3713	1				
1/2-x,1/2+y	0.1548	0.7907	0.1287	1				
1/2-x,1/2-y	0.1548	0.2093	0.6287	1				
1/2+x,1/2-y	0.8452	0.2093	0.8713	1				
x=	0.3452							
y=	0.2907							
z=	0.3713							

15ffff C2/c
64 CARBTC07

a=	20.1818		
b=	11.3504	b/a=	0.5624077
c=	19.7616	c/a=	0.9791793
alpha=	90	alpha=	90
beta=	111.463	beta=	111.463
gamma=	90	gamma=	90

Matrix Representation

1	0	-0.358282
0	0.5624077	0
0	0	0.9112771
a	b	c
1	0.5624077	0.9791793
90	111.463	90
alpha	beta	gamma

See #63 above.

f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of neare Center of Mass Coordinates
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest
next neighbors >40% of nearest
f: 1 nearest neighbor
12 neighbors within 25% of nearest

f 1				
x,y,z	0.0948	0.0343	0.3766	1
1-x,y,1/2-z	0.9052	0.0343	0.1234	1
1-x,1-y,1-z	0.9052	0.9657	0.6234	1
x,1-y,1/2+z	0.0948	0.9657	0.8766	1
1/2+x,1/2+	0.5948	0.5343	0.3766	1

next neighbors >40% of nearest	1/2-x,1/2+y	0.4052	0.5343	0.1234	1
sphere packing	1/2-x,1/2-y	0.4052	0.4657	0.6234	1
	1/2+x,1/2-y	0.5948	0.4657	0.8766	1
See above.	x=	0.0948			
	y=	0.0343			
	z=	0.3766			
	f 1				
	x,y,z	0.3793	0.0648	0.1221	1
	1-x,y,1/2-z	0.6207	0.0648	0.3779	1
	1-x,1-y,1-z	0.6207	0.9352	0.8779	1
	x,1-y,1/2+z	0.3793	0.9352	0.6221	1
	1/2+x,1/2+y	0.8793	0.5648	0.1221	1
	1/2-x,1/2+y	0.1207	0.5648	0.3779	1
	1/2-x,1/2-y	0.1207	0.4352	0.8779	1
	1/2+x,1/2-y	0.8793	0.4352	0.6221	1
	x=	0.3793			
	y=	0.0648			
	z=	0.1221			
	f 1				
	x,y,z	0.1267	0.3131	0.1231	1
	1-x,y,1/2-z	0.8733	0.3131	0.3769	1
	1-x,1-y,1-z	0.8733	0.6869	0.8769	1
	x,1-y,1/2+z	0.1267	0.6869	0.6231	1
	1/2+x,1/2+y	0.6267	0.8131	0.1231	1
	1/2-x,1/2+y	0.3733	0.8131	0.3769	1
	1/2-x,1/2-y	0.3733	0.1869	0.8769	1
	1/2+x,1/2-y	0.6267	0.1869	0.6231	1
	x=	0.1267			
	y=	0.3131			
	z=	0.1231			
	f 1				
	x,y,z	0.3418	0.285	0.3745	1
	1-x,y,1/2-z	0.6582	0.285	0.1255	1
	1-x,1-y,1-z	0.6582	0.715	0.6255	1
	x,1-y,1/2+z	0.3418	0.715	0.8745	1
	1/2+x,1/2+y	0.8418	0.785	0.3745	1
	1/2-x,1/2+y	0.1582	0.785	0.1255	1
	1/2-x,1/2-y	0.1582	0.215	0.6255	1
	1/2+x,1/2-y	0.8418	0.215	0.8745	1
	x=	0.3418			
	y=	0.285			
	z=	0.3745			

Triclinic Crystal Structures (1-2)

2i P_-1

65 BASXOI

a=	9.1472		
b=	10.4952	b/a=	1.1473675
c=	10.5082	c/a=	1.1487887
alpha=	85.60	alpha=	85.602
beta=	89.83	beta=	89.832
gamma=	65.71	gamma=	65.713

2 neighbors within 1% of nearest
next neighbor 14% farther than nearest

Square packing of p-1 rods.

Matrix Representation

1	0.4719209	0.0033684
0	1.0458216	0.0951276
0	0	1.1448384

a	b	c
1	1.1473675	1.1487887
85.602	89.832	65.713
alpha	beta	gamma

Center of Mass Coordinates

i 1

i	x,y,z	0.2974607	0.3063664	0.7986807	1
ii	1-x,1-y,1-z	-0.297461	0.6936336	1.2013193	1
	x=	0.2974607			
	y=	0.3063664			
	z=	0.7986807			

Molecular 3-fold axes

i 1

i	x,y,z	0.183	0.1363	0.8126	1
ii	x,y,z	-0.183	0.8637	1.1874	1
	x=	0.183			
	y=	0.1363			
	z=	0.8126			

Transformation to Rod Coordinates

0.615286	0.071184	1	0
0.384714	-0.071184	-1	0.5
0	1	0	1
0	0	0	1

Det= 1

Inverse Transformation

1	1	0	-0.5
0	0	1	-1
0.384714	-0.615286	-0.071184	0.378827
0	0	0	1

Det= 1

rod axis:

1	-1	0

rod origin:

0	0.5	1

Transformation to monoclinic axes:

-0.384714
0.071184

Transformation to Orthogonal Coordinates

1	-0.051402326	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0.051402326	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Transformation to orthogonal axes:

-0.051402326

Rotation about rod and rescaling:

0.385523889	1.064837859	0	0
-0.830277535	0.300601469	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

0.300601469	-1.064837859	0	0
0.830277535	0.385523889	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

70.09724248 degrees

Rescaling parameter:

1.132478845

Matrix Representation

0.307201	0.8485059	0.528079
0.155112	0.428429472	-1.045822
-0.950534	0.344140092	0

a	b	c
1.010914	1.010913685	1.171585
89.99916	89.99963973	90
alpha	beta	gamma

p-1 (#2)

c 1

x,y,z	0.242472	6.36615E-09	0.247908	1
-x,-y,-z	-0.242472	-6.36615E-09	-0.247908	1

c 1

x,y,z	0.142336	-0.230276221	0.307522	1
-x,-y,-z	-0.142336	0.230276221	-0.307522	1

Z'= 1

	|G|	Z	|G|/Z	
Daughter 2i	2	2	1	
Rod 2c	2	1	2	
		2	2	
		(size)	(index)	

2i P_-1

66 XAGXAE

a=	9.007214		
b=	9.208015	b/a=	1.0222934
c=	9.1952	c/a=	1.0208706
alpha=	92.502	alpha=	92.502
beta=	100.722	beta=	100.722
gamma=	109.8421	gamma=	109.84211

2 neighbors within 6% of nearest
next neighbor 11% farther than nearest

Oblique packing of p-1 rods.

Matrix Representation

1	-0.346996	-0.189927
0	0.9616014	-0.115914
0	0	0.9963276

a	b	c
1	1.0222934	1.0208706
92.502	100.722	109.84211
alpha	beta	gamma

Center of Mass Coordinates

i 1

i	x,y,z	0.1543118	0.2575931	-0.184303	1
ii	1-x,1-y,1-z	-0.154312	0.7424069	0.1843034	1
	x=	0.1543118			
	y=	0.2575931			
	z=	-0.184303			

Molecular 3-fold axes

i 1

i	x,y,z	0.2624	0.0892	-0.1867	1
ii	x,y,z	-0.2624	0.9108	0.1867	1
	x=	0.2624			
	y=	0.0892			
	z=	-0.1867			

Transformation to Rod Coordinates

0	1	0	0
0.043593	0.332027	1	0
1	0	0	0
0	0	0	1

Det= 1

Inverse Transformation

0	0	1	0
1	0	0	0
-0.332027	1	-0.043593	0
0	0	0	1

Det= 1

rod axis:

0	1	0

rod origin:

0	0	0

Transformation to monoclinic axes:

0.332027
0.043593

Transformation to Orthogonal Coordinates

1	0.197125158	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	-0.197125158	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Transformation to orthogonal axes:

0.197125158

Rotation about rod and rescaling:

-0.796749907	-0.51590333	0	0
0.5726109	-0.884327847	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

-0.884327847	0.51590333	0	0
-0.5726109	-0.796749907	0	0
0	0	1	0
0	0	0	1

Det= 1

rotation angle:

-147.0765496

Rescaling parameter:

0.949192636

Matrix Representation

0.64687	-0.640909051	-0.346996
0.233425	-0.231273599	0.961601
-0.681362	-0.687691794	0

a	b	c
0.968082	0.968076387	1.022293
89.99999	90.00000241	90.00014
alpha	beta	gamma

p-1 (#2)

c 1

x,y,z	0.269495	4.31622E-06	0.214392	1
-x,-y,-z	-0.269495	-4.31622E-06	0.785608	1

c 1

x,y,z	0.346219	-0.072542055	0.010215	1
-x,-y,-z	-0.346219	0.072542055	0.989785	1

Z'= 1

	|G|	Z	|G|/Z	
Daughter 2i	4	2	2	
Rod 2c	2	1	2	
		2	1	
		(size)	(index)	

2i P_-1

67 MEZDIE01

a=	9.920097		
b=	14.51031	b/a=	1.4627186
c=	9.135857	c/a=	0.9209443
alpha=	90.47694	alpha=	90.47694
beta=	111.6724	beta=	111.67244

Matrix Representation

1	0.0003125	-0.340105
0	1.4627185	-0.007593
0	0	0.8558094

a	b	c
1	1.4627186	0.9209443

Transformation to Reduced Cell

0.5	0.5	0	0.75
0.5	-0.5	0	0.25
0.5	0.5	-1	0.25
0	0	0	1

Det= 0.5

Matrix Representation

0.330103967	0.329791489	0.340104544
0.727562585	-0.735155941	0.007593356
0.427904687	0.427904687	-0.855809373

a	b	c
0.906321337	0.912315244	0.920944321

		|G|	Z	|G|/Z
Daughter	2i	2	2	1
Ref. Lattice	BCC	48	1	48
			2	48
			(size)	(index)

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

gamma= 89.98776 gamma= 89.98776 90.47694 111.67244 89.98776
alpha beta gamma

6 neighbors within 3% of nearest
next neighbor 11% farther than nearest
sphere packing

Inverse Transformation

1	1	0	-1
1	-1	0	-0.5
1	0	-1	-0.5
0	0	0	1

Det= 2

107.9992896 107.3143809 107.0838036
alpha beta gamma

Normalized Niggli Matrix

1	1.01327063	1.032529194
-0.316067389	-0.302416346	-0.295712962

Reduced Cell

Character	44 (aP)	… but close to 5 (cI)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

Overall Transformation

0.5	-1	-0.5	0
0.5	1	-0.5	-0.5
0.5	0	0.5	-0.5
0	0	0	1

Det= 1

Center of Mass Coordinates

i	1			
x,y,z	0.7605859	0.2506235	0.24179	1
1-x,1-y,1-z	0.2394141	0.7493765	0.7582	1

x= 0.7605859
y= 0.2506235
z= 0.24179

0,0,0 0.011209412 0.009962353 0.018795882 1
-0.011209412 -1.009962353 -1.018795882 1

Z'= 1

Order Parameter = Coupled

2i P_-1

Matrix Representation

1	-0.000126	-0.341044
0	1.4610255	-0.008613
0	0	0.8556222

68 MEZDOK01
a= 9.944575
b= 14.52928 b/a= 1.4610255
c= 9.160215 c/a= 0.9211268
alpha= 90.53393 alpha= 90.53393
beta= 111.7308 beta= 111.73083
gamma= 90.00494 gamma= 90.00494

a	b	c
1	1.4610255	0.9211268
90.53393	111.73083	90.00494
alpha	beta	gamma

See #67 above.

6 neighbors within 3% of nearest
next neighbor 11% farther than nearest
sphere packing

See above.

Center of Mass Coordinates

i	1			
x,y,z	0.7617465	0.2495818	0.2417818	1
1-x,1-y,1-z	0.2382535	0.7504182	0.7582182	1

x= 0.7617465
y= 0.2495818
z= 0.2417818

2i P_-1

69 XUWROW **Thin Film Crystal w/ Large Voids**

a= 9.6802
b= 17.9373 b/a= 1.852989
c= 28.0315 c/a= 2.895756
alpha= 96.622
beta= 99.962
gamma= 105.681

i 1
0.041217 0.745871 0.4152899 x,y,z
0.958783 0.254129 0.5847101 1-x,1-y,1-z

x= 0.041217
y= 0.745871
z= 0.41529

Molecules clustered near c=(n+1)/2 and large c/a lead to unrealistically large gaps between layers.

2iii P_-1

Matrix Representation

1	0.0018522	0.0015842
0	1.4884328	0.0017618
0	0	2.5714065

70 OHABEE
a= 9.79238
b= 14.57531 b/a= 1.488434
c= 25.1802 c/a= 2.5714076
alpha= 89.9607 alpha= 89.9607
beta= 89.9647 beta= 89.9647
gamma= 89.9287 gamma= 89.9287

a	b	c	
1	1.488434	2.5714076	
89.9607	89.9647	89.9287	
alpha	beta	gamma	

Transformation to Reduced Cell

-0.333333	-0.333333	-0.333333	0.333333
0	0.5	-0.5	-0.25
-0.333333	0.166667	0.166667	0.083333
0	0	0	1

Det= -0.166667

Inverse Transformation

-1	1	1	-0.5
-1	0	-2	1.5
-1	-1	1	0
0	0	0	1

Det= 6

Matrix Representation

-0.333861416	-0.332143174	-0.33399541
-0.000587265	0.744510039	-0.743922774
-0.857135491	0.428567745	0.428567745

a	b	c		
0.919861424	0.921023669	0.921218943		
107.7916146	107.5410774	107.6508078		
alpha	beta	gamma		
Daughter	2iii	2	6	0.333333
Ref. Lattice	BCC	48	1	48
			6	144
			(size)	(index)

Reduced Cell

Character	44 (aP)	… but close to 5 (cI)	
Type	II		
b.b≥a.a	True	|b.c|≤b.b/2	True
c.c≥b.b	True	|a.c|≤a.a/2	True
2|D+E+F| ≤ A+B	True	|a.b|≤a.a/2	True

Transformation to Conventional Cell

0	1	1	0
1	0	1	0
1	1	0	0
0	0	0	1

Det= 2

Overall Transformation

-0.5	0	2	0
-0.5	-1	-1	0
-0.5	1	-1	0.5
0	0	0	1

Det= -3

Center of Mass Coordinates

i: 1 nearest neighbor
8 neighbors within 10% of nearest
next neighbor 16% farther than nearest

i	1			
x,y,z	0.3198117	0.2466519	0.5851674	1
1-x,1-y,1-z	0.6801883	0.7533481	0.4148326	1

x= 0.3198117
y= 0.2466519
z= 0.5851674

0,0,0 0.012007596 0.009853611 0.018703811 1
-0.012007596 -0.009853611 -1.018703811 1

Z'= 1

Order Parameter = Coupled

error 0.012007596 0.009853611 0.018703811

i: 1 nearest neighbor
8 neighbors within 10% of nearest
next neighbor 18% farther than nearest

i				
x,y,z	0.016409	0.2535574	0.2500246	1
1-x,1-y,1-z	0.983591	0.7464426	0.7499754	1

x= 0.016409
y= 0.2535574
z= 0.2500246

-0.012827038 0.983541861 -0.019941823 1
0.012827038 -0.983541861 -0.980058177 1

error -0.012827038 -0.016458139 -0.019941823

i: 2 nearest neighbors
8 neighbors within 10% of nearest
next neighbor 15% farther than nearest
sphere packing

i				
x,y,z	0.3180757	0.7535794	0.0817532	1
1-x,1-y,1-z	0.6819243	0.2464206	0.9182468	1

x= 0.3180757
y= 0.7535794
z= 0.0817532

0.017256975 1.018417871 -0.989901882 1
-0.017256975 -1.018417871 -0.010098118 1

error 0.017256975 0.018417871 0.010098118

2iii P_-1

Matrix Representation

1	0.0307136	-0.006985
0	0.9181114	0.0164553
0	0	0.4795676

71 CANFOM
a= 18.4086
b= 16.9106 b/a= 0.918625
c= 8.8343 c/a= 0.4799007
alpha= 88.064 alpha= 88.064
beta= 90.834 beta= 90.834
gamma= 88.084 gamma= 88.084

a	b	c	
1	0.918625	0.4799007	
88.064	90.834	88.084	
alpha	beta	gamma	

Transformation to Planar Coordinates

0.006985	-0.030726	1	0.25
0	1	0	0
1	0	0	0.25
0	0	0	1

Det= -1

Inverse Transformation

0	0	1	-0.25
0	1	0	0
1	0.030726	-0.006985	-0.248254
0	0	0	1

Det= -1

Rotation about plane normal and rescaling:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Inverse Transformation

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Det= 1

Matrix Representation

-3.90214E-08	-1.29356E-05	1
0.0164553	0.918111404	0
0.479567629	0	0

a	b	c
0.479849859	0.918111404	1
90.00080726	90.00000466	88.03479
alpha	beta	gamma

		|G|	Z	|G|/Z
Daughter	2iii	2	8	0.25
Plane	2_1	2	4	0.5
		2	2	
		(size)	(index)	

pg (#4) in projection
distorted p6mm (#17) - puckered honeycomb
2_1 when accounting for 3rd dimension

i: 1 nearest neighbor
3 neighbors within 8% of nearest
next neighbor 26% farther than nearest
i: 1 nearest neighbor
3 neighbors within 8% of nearest
next neighbor 29% farther than ne
i: 1 nearest neighbor
3 neighbors within 7% of nearest
next neighbor 33% farther than nearest
i: 1 nearest neighbor
3 neighbors within 9% of nearest
next neighbor 32% farther than ne

Center of Mass Coordinates

i	1			
x,y,z	0.1987578	0.0060756	0.5133267	1
1-x,1-y,1-z	0.8012422	0.9939244	0.4866733	1

x= 0.1987578
y= 0.0060756
z= 0.5133267

i	1			
x,y,z	0.2997033	0.5063144	0.9700989	1
1-x,1-y,1-z	0.7002967	0.4936856	0.0299011	1

planar

plane normal:

1	0	0

plane origin:

0.25	0	0.25

Transformation to orthogonal axes:

0.006985		
-0.030726		

rotation angle:

0 degrees

1/4,0,-z 0.263326667 0.006075556 -0.052895 1
0.236673333 0.993924444 0.580129 1

3/4,1/2,z 0.720098889 0.506314444 0.060231 1
-0.220098889 0.493685556 0.467003 1

z= 0.056562756
error= 0.013326667 0.006075556 0.003668

Z'= 4

x= 0.2997033
y= 0.5063144
z= 0.9700989

i 1

x,y,z	0.12601	0.6773511	0.4547744	1	
1-x,1-y,1-z	0.87399	0.3226489	0.5452256	1	

x= 0.12601
y= 0.6773511
z= 0.4547744

i 1

x,y,z	0.3692444	0.1746478	0.0148856	1	
1-x,1-y,1-z	0.6307556	0.8253522	0.9851144	1	

x= 0.3692444
y= 0.1746478
z= 0.0148856

	-0.029901111	0.006314444	0.003668	

1/4,2/3,z	0.204774444	0.677351111	-0.104608	1
	0.295225556	0.322648889	0.631842	1
3/4,1/6,-z	-0.235114444	0.174647778	0.126253	1
	0.735114444	0.825352222	0.400981	1

z=	0.115430415			
error=	-0.045225556	0.010684444	0.010823	
	0.014885556	0.007981111	0.010823	

R. B. McClurg, July, 2008

Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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

Table 7: Neighbor Histogram

Neighbor distances scaled to the nearest neighbor distance
Red entries highlight large steps in the histogram

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Dimers																		
	205c	FOJBUB02																
monomer	c	1.000	1.329	1.329	1.329	1.329	1.329	1.329	1.449	1.449	1.449	1.449	1.449	1.449	1.966	1.966	1.966	2.121
dimer	a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414
	205c	VADRAU																
monomer	c	1.000	1.250	1.250	1.250	1.250	1.250	1.250	1.377	1.377	1.377	1.377	1.377	1.377	1.860	1.860	1.860	2.039
dimer	a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414
	88f	LUFYEQ																
monomer	f	1.000	1.331	1.331	1.563	1.563	1.568	1.573	1.573	1.582	1.582	1.597	1.650	1.650	2.082	2.082	2.089	2.089
dimer	e	1.000	1.126	1.126	1.270	1.270	1.270	1.270	1.482	1.482	1.562	1.562	1.562	1.562	1.689	1.989	1.989	2.032
quatramer	a	1.000	1.000	1.000	1.000	1.600	1.600	1.600	1.600	1.600	1.600	1.600	1.600	1.697	1.697	1.697	1.697	1.801
	14e	CARBTC																
monomer	e	1.000	1.060	1.060	1.114	1.114	1.207	1.207	1.231	1.231	1.245	1.245	1.264	1.438	1.438	1.632	1.688	1.727
dimer	a	1.000	1.000	1.000	1.000	1.062	1.062	1.672	1.672	1.695	1.695	1.760	1.760	1.760	1.760	1.804	1.804	1.981
Rods																		
	137a	FUZTEZ																
	a	1.000	1.000	1.123	1.123	1.123	1.123	1.123	1.123	1.123	1.123	1.422	1.422	1.422	1.422	1.739	1.739	1.739
	62c	GUTCED																
	c	1.000	1.000	1.106	1.106	1.174	1.174	1.218	1.218	1.218	1.218	1.321	1.321	1.539	1.539	1.680	1.680	1.697
	62c	JEYSEL																
	c	1.000	1.000	1.125	1.125	1.203	1.203	1.353	1.353	1.430	1.430	1.521	1.521	1.521	1.521	1.647	1.647	1.647
	62c	RIMMOP																
	c	1.000	1.000	1.042	1.042	1.171	1.171	1.210	1.210	1.255	1.255	1.324	1.324	1.324	1.324	1.687	1.687	1.687
	15e	BOGMEP																
	e	1.000	1.000	1.105	1.105	1.117	1.117	1.151	1.151	1.267	1.267	1.267	1.267	1.515	1.515	1.533	1.533	1.787
	15e	MSISUL10																
	e	1.000	1.000	1.191	1.191	1.463	1.463	1.473	1.473	1.491	1.491	1.491	1.491	1.564	1.564	1.661	1.661	1.867
	15e	TMGEHS10																
	e	1.000	1.000	1.195	1.195	1.468	1.468	1.477	1.477	1.499	1.499	1.499	1.499	1.549	1.549	1.668	1.668	1.852
	15e	TMSNHS10																
	e	1.000	1.000	1.213	1.213	1.497	1.497	1.513	1.513	1.525	1.525	1.525	1.525	1.557	1.557	1.678	1.678	1.850
	14e	DOCNIS																
	e	1.000	1.030	1.102	1.102	1.125	1.125	1.161	1.161	1.222	1.224	1.224	1.247	1.532	1.532	1.551	1.551	1.768
	14e	TMSIAD																
	e	1.000	1.036	1.238	1.238	1.248	1.277	1.347	1.347	1.392	1.392	1.470	1.470	1.496	1.496	1.919	1.919	1.955
	2i	BASXOI																
	i	1.000	1.010	1.144	1.147	1.270	1.294	1.316	1.316	1.509	1.509	1.511	1.511	1.531	1.541	1.541	1.735	1.777
	11e	MECKIO																
	e	1.000	1.000	1.022	1.022	1.122	1.122	1.152	1.152	1.188	1.188	1.206	1.206	1.329	1.329	1.624	1.624	1.647
	13efg	RIMNAC																
	e	1.000	1.000	1.019	1.019	1.049	1.049	1.094	1.094	1.172	1.172	1.174	1.174	1.245	1.245	1.644	1.644	1.660
	f	1.000	1.000	1.019	1.019	1.031	1.031	1.038	1.038	1.172	1.172	1.172	1.172	1.421	1.421	1.461	1.461	1.644
	g	1.000	1.007	1.007	1.038	1.041	1.045	1.056	1.102	1.172	1.180	1.182	1.207	1.254	1.431	1.471	1.629	1.655
	14ee	MXSNOX																
	e	1.000	1.003	1.043	1.155	1.384	1.473	1.483	1.483	1.484	1.492	1.492	1.524	1.566	1.566	1.582	1.604	1.758
	e	1.000	1.003	1.043	1.058	1.384	1.420	1.473	1.484	1.524	1.540	1.566	1.566	1.582	1.758	1.767	1.805	1.805
	2i	XAGXAE																
	i	1.000	1.058	1.112	1.149	1.324	1.467	1.467	1.498	1.498	1.500	1.500	1.514	1.539	1.706	1.706	1.829	1.853
	14e	QUGBOJ																
	e	1.000	1.010	1.014	1.014	1.099	1.099	1.109	1.109	1.258	1.266	1.286	1.286	1.464	1.464	1.488	1.488	1.679
Planes																		
	19a	MZNMOX10																
	a	1.000	1.000	1.026	1.026	1.132	1.132	1.151	1.151	1.268	1.268	1.421	1.421	1.432	1.432	1.432	1.432	1.595
	14e	CAMPOV																
	e	1.000	1.035	1.035	1.262	1.262	1.264	1.300	1.300	1.316	1.345	1.345	1.468	1.468	1.475	1.837	1.837	1.850

14e	VAVYAS																
e	1.000	1.038	1.038	1.266	1.266	1.290	1.290	1.303	1.375	1.392	1.392	1.526	1.526	1.539	1.852	1.852	1.873
14ee	CANFIG																
e	1.000	1.044	1.055	1.275	1.395	1.521	1.521	1.590	1.633	1.633	1.690	1.707	1.707	1.744	1.893	1.893	1.936
e	1.000	1.044	1.055	1.302	1.395	1.521	1.521	1.590	1.690	1.744	1.773	1.773	1.818	1.818	1.853	1.853	1.893
2iiii	CANFOM																
i	1.000	1.056	1.072	1.264	1.363	1.523	1.523	1.604	1.614	1.676	1.679	1.695	1.721	1.723	1.913	1.918	1.961
i	1.000	1.071	1.073	1.293	1.449	1.547	1.547	1.631	1.639	1.702	1.721	1.739	1.750	1.814	1.870	1.937	1.960
i	1.000	1.054	1.056	1.333	1.363	1.523	1.523	1.606	1.712	1.721	1.752	1.781	1.789	1.815	1.823	1.824	1.854
i	1.000	1.073	1.089	1.315	1.449	1.547	1.547	1.629	1.705	1.780	1.809	1.814	1.817	1.843	1.852	1.852	1.852
Sphere Packings																	
227a	ZNOXAC01																
a	1.000	1.000	1.000	1.000	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.633	1.915
217a	DEQPAQ																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	HMSIPA																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	HXMTAM07																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	KELREY																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	MESIAD																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	MPTHOT01																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	NIWMIP																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	POSLOY10																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	TMEPTC																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a	YEYQAU																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
217a*	HMGETP																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.155	1.155	1.155	1.155	1.155	1.155	1.633	1.633	1.633
215a	FOHCUA																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414
215a	FUZVOL																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414
215a*	JUFWUC																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414	1.414
176h	CUCZUV																
h	1.000	1.000	1.022	1.022	1.067	1.067	1.067	1.067	1.137	1.137	1.140	1.140	1.492	1.492	1.492	1.492	1.562
165d	DILWIE01																
d	1.000	1.000	1.000	1.035	1.035	1.035	1.059	1.059	1.059	1.059	1.059	1.059	1.456	1.456	1.456	1.481	1.481
165d	ZEYHIU																
d	1.000	1.000	1.000	1.091	1.091	1.091	1.094	1.094	1.094	1.094	1.094	1.094	1.482	1.482	1.482	1.545	1.545
161a	TCYMET																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.042	1.042	1.167	1.167	1.167	1.167	1.167	1.167	1.624	1.624	1.624
147d	ZIZHIZ																
d	1.000	1.000	1.000	1.010	1.010	1.010	1.055	1.055	1.055	1.055	1.055	1.055	1.454	1.454	1.454	1.461	1.461
152b	MTRETC10																
b	1.000	1.000	1.010	1.010	1.010	1.010	1.010	1.010	1.071	1.071	1.071	1.071	1.421	1.421	1.421	1.421	1.521
141a	FUZLUH																
a	1.000	1.000	1.000	1.000	1.358	1.358	1.386	1.386	1.386	1.386	1.493	1.493	1.493	1.493	1.493	1.493	1.493
141a	VAFWAA																
a	1.000	1.000	1.000	1.000	1.351	1.351	1.383	1.383	1.383	1.383	1.493	1.493	1.493	1.493	1.493	1.493	1.493
121a	ZZZKDW01																
a	1.000	1.000	1.000	1.000	1.028	1.028	1.028	1.028	1.028	1.028	1.028	1.028	1.414	1.414	1.414	1.414	1.491
142a	KUJSIR																

a	1.000	1.000	1.000	1.000	1.006	1.006	1.006	1.006	1.006	1.006	1.006	1.006	1.414	1.414	1.414	1.414	1.431
120b	YEMRIR																
b	1.000	1.000	1.000	1.000	1.062	1.062	1.414	1.414	1.414	1.414	1.458	1.458	1.458	1.458	1.458	1.458	1.458
114a	ADAMAN08																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.025	1.025	1.025	1.025	1.377	1.377	1.450	1.450	1.450
114a	GERHOA																
a	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.063	1.063	1.063	1.063	1.320	1.320	1.503	1.503	1.503
88a	KANGUB01																
a	1.000	1.000	1.000	1.000	1.111	1.111	1.111	1.111	1.414	1.414	1.414	1.414	1.495	1.495	1.495	1.495	1.495
64d,f	Methane																
d	1.000	1.000	1.034	1.034	1.034	1.034	1.040	1.040	1.042	1.042	1.082	1.082	1.462	1.462	1.462	1.462	1.478
f	1.000	1.000	1.037	1.037	1.038	1.038	1.040	1.040	1.042	1.042	1.082	1.082	1.345	1.465	1.469	1.481	1.481
60c,d	YIMWEW																
c	1.000	1.000	1.010	1.010	1.041	1.041	1.049	1.049	1.117	1.117	1.213	1.213	1.325	1.325	1.569	1.569	1.641
d	1.000	1.010	1.013	1.013	1.040	1.040	1.049	1.071	1.071	1.117	1.213	1.243	1.288	1.288	1.564	1.569	1.641
15e	RASDOE																
e	1.000	1.000	1.014	1.014	1.018	1.018	1.124	1.124	1.124	1.124	1.235	1.235	1.241	1.241	1.592	1.592	1.609
15e	TFMETH02																
e	1.000	1.000	1.018	1.018	1.059	1.059	1.118	1.118	1.118	1.118	1.198	1.198	1.313	1.313	1.533	1.533	1.697
15e	REKYUB																
e	1.000	1.000	1.042	1.042	1.088	1.088	1.131	1.131	1.159	1.159	1.159	1.159	1.411	1.411	1.477	1.477	1.750
12i	MECKOU																
i	1.000	1.003	1.003	1.003	1.003	1.034	1.083	1.083	1.146	1.146	1.182	1.182	1.400	1.475	1.548	1.548	1.570
14e	MECKUA																
e	1.000	1.000	1.000	1.000	1.009	1.009	1.076	1.083	1.112	1.112	1.131	1.138	1.454	1.454	1.495	1.495	1.536
14e	TOHSUE																
e	1.000	1.000	1.000	1.001	1.001	1.001	1.011	1.012	1.012	1.012	1.024	1.024	1.398	1.398	1.439	1.439	1.439
15ffff	CARBTC07																
f	1.000	1.005	1.062	1.086	1.141	1.155	1.198	1.212	1.213	1.220	1.220	1.237	1.439	1.492	1.592	1.594	1.737
f	1.000	1.071	1.100	1.119	1.150	1.166	1.167	1.174	1.209	1.223	1.226	1.228	1.411	1.505	1.606	1.630	1.747
f	1.000	1.056	1.079	1.096	1.150	1.166	1.167	1.206	1.223	1.229	1.231	1.231	1.409	1.599	1.599	1.652	1.675
f	1.000	1.046	1.069	1.090	1.141	1.155	1.164	1.195	1.215	1.217	1.219	1.237	1.436	1.495	1.495	1.611	1.732
15ffff	CTBROM																
f	1.000	1.016	1.062	1.085	1.123	1.154	1.188	1.197	1.203	1.203	1.205	1.219	1.418	1.500	1.588	1.591	1.727
f	1.000	1.085	1.108	1.141	1.141	1.169	1.179	1.184	1.213	1.223	1.224	1.241	1.432	1.532	1.614	1.625	1.763
f	1.000	1.066	1.093	1.108	1.141	1.169	1.184	1.207	1.228	1.230	1.242	1.245	1.414	1.616	1.616	1.659	1.670
f	1.000	1.044	1.070	1.085	1.124	1.154	1.155	1.182	1.199	1.203	1.216	1.216	1.464	1.486	1.486	1.585	1.727
2i	MEZDIE01																
i	1.000	1.010	1.010	1.014	1.021	1.021	1.108	1.108	1.172	1.175	1.198	1.198	1.218	1.227	1.619	1.621	1.621
2i	MEZDOK01																
i	1.000	1.006	1.007	1.016	1.021	1.021	1.108	1.108	1.167	1.175	1.197	1.197	1.221	1.225	1.615	1.619	1.619
2i	XUWROW																
i	1.000	1.000	1.041	1.074	1.114	1.413	1.521	1.711	1.843	1.853	1.853	1.853	1.853	2.000	2.000	2.330	2.330
2iii	OHABEE																
i	1.000	1.006	1.007	1.015	1.018	1.033	1.094	1.094	1.168	1.169	1.183	1.185	1.186	1.212	1.611	1.623	1.629
i	1.000	1.002	1.002	1.005	1.008	1.009	1.096	1.096	1.186	1.188	1.189	1.215	1.215	1.216	1.623	1.624	1.632
i	1.000	1.000	1.005	1.009	1.020	1.028	1.096	1.096	1.160	1.171	1.178	1.186	1.215	1.216	1.614	1.627	1.632
Mixed																	
218ac	KOXKOX																
a	1.000	1.000	1.118	1.118	1.118	1.118	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.803	1.803	1.803
c	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.549	1.549	1.549	1.549	1.549
218ac	RUQMEV																
a	1.000	1.000	1.118	1.118	1.118	1.118	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.803	1.803	1.803
c	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.549	1.549	1.549	1.549	1.549
218ac	SENLAY																
a	1.000	1.000	1.118	1.118	1.118	1.118	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.225	1.803	1.803	1.803
c	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.549	1.549	1.549	1.549	1.549

Molecular Crystal Global Phase Diagrams: II. Reference Lattices

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

Table 8: Order Parameters

Order Parameters Calculated Using:
COPL as found on:
H.T.Stokes and D.M.Hatch, (2002). ISOTROPY, stokes.byu.edu/isotropy.html.

Sphere Packings:

ZNOXAC01
Parent: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
Subgroup: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	227 Fd-3m	1

GM1+ is the primary OP.

DEQPAQ, et al.
Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup: 217 Td-3, I-43m, I-43m
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	229 Im-3m	1
GM2-	(a)	217 I-43m	1

GM2- is the primary OP.

FOHCUA, et al.
Parent: 221 Oh-1, Pm-3m, P4/m-32/m
Subgroup: 215 Td-1, P-43m, P-43m
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	221 Pm-3m	1
GM2-	(a)	215 P-43m	1

GM2- is the primary OP.

CUCZUV
Parent: 194 D6h-4, P6_3/mmc, P6_3/m2/m2/c
Subgroup: 176 C6h-2, P6_3/m, P6_3/m
Lattice vectors:
1 -1 0
1 2 0
0 0 1
origin: 0 0 1/2

Irrep	Dir	Subgroup	Size
GM1+	(a)	194 P6_3/mmc	1
GM2+	(a)	176 P6_3/m	1
K1	(a,0)	193 P6_3/mcm	3
K4	(a,0)	176 P6_3/m	3

K4 is the primary OP.

DILWIE01 & ZEYHIU

Parent: 194 D6h-4, P6_3/mmc, P6_3/m2/m2/c
Subgroup: 165 D3d-4, P-3c1, P-32/c1
Lattice vectors:
1 0 0
0 1 0
0 0 2
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	194 P6_3/mmc	1
GM3+	(a)	164 P-3m1	1
A2	(a,a)	165 P-3c1	2

A2 is the primary OP.

TCYMET

Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup: 161 C3v-6, R3c, R3c, hexangonal axes
Lattice vectors:
0 1 -1
-1 0 1
1 1 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	229 Im-3m	1
GM5+	(a,a,a)	166 R-3m	1
GM2-	(a)	217 I-43m	1
GM4-	(a,a,a)	160 R3m	1
H2+	(a)	223 Pm-3n	2
H4+	(a,a,a)	167 R-3c	2
H1-	(a)	222 Pn-3n	2
H5-	(a,a,a)	167 R-3c	2

Coupled OP.

ZIZHIZ

Parent: 194 D6h-4, P6_3/mmc, P6_3/m2/m2/c
Subgroup: 147 C3i-1, P-3, P-3
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	194 P6_3/mmc	1
GM2+	(a)	176 P6_3/m	1
GM3+	(a)	164 P-3m1	1
GM4+	(a)	163 P-31c	1

Coupled OP.

MTRETC10

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 152 D3-4, P3_121, P3_121
Lattice vectors:
0 -1/2 -1/2
1/2 0 1/2
-1 -1 1
origin: -1/6 1/6 -1/2

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	225 Fm-3m	1
GM5+		(a,-a,-a)	166 R-3m	1
GM1-		(a)	209 F432	1
GM5-		(a,-a,-a)	155 R32	1
LD3	2/3	(0,0,0,0,0,0,a,0,0,0,0,0,0,0,-1.732a,0)	152 P3_121	3

LD3 is the primary OP.

FUZLUH & VAFWAA

Parent: 227 Oh-7, Fd-3m, F4_1/d-32/m, origin choice 2
Subgroup: 141 D4h-19, I4_1/amd, I4_1/a2/m2/d, origin choice 2
Lattice vectors:
1/2 -1/2 0
1/2 1/2 0
0 0 1
origin: 1/4 1/4 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	227 Fd-3m	1
GM3+	(a,0)	141 I4_1/amd	1

GM3+ is the primary OP.

ZZZKNW01

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 121 D2d-11, I-42m, I-42m
Lattice vectors:
-1/2 0 1/2
1/2 0 1/2
0 1 0
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM3+	(a,-1.732a)	139 I4/mmm	1
GM5-	(0,0,a)	121 I-42m	1

GM5- is the primary OP.

KUJSIR

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 142 D4h-20, I4_1/acd, I4_1/a2/c2/d, origin choice 2
Lattice vectors:
1 0 0
0 0 -1
0 2 0
origin: 0 1/4 1/4

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM3+	(a,-1.732a)	139 I4/mmm	1
X4-	(a,0,0)	134 P4_2/nnm	2
W3	(0,0,a,a,0,0)	142 I4_1/acd	4

W3 is the primary OP.

YEMRIR

Parent: 221 Oh-1, Pm-3m, P4/m-32/m
Subgroup: 120 D2d-10, I-4c2, I-4c2
Lattice vectors:
1 -1 0
1 1 0
0 0 2
origin: -1/2 -1/2 -1/2

Irrep	Dir	Subgroup	Size
GM1+	(a)	221 Pm-3m	1
GM3+	(a,0)	123 P4/mmm	1
GM2-	(a)	215 P-43m	1
GM3-	(a,0)	111 P-42m	1
R4+	(a,0,0)	140 I4/mcm	2
R5-	(a,0,0)	140 I4/mcm	2

Coupled OP.

ADAMAN08 & GERHOA

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 114 D2d-4, P-42_1c, P-42_1c
Lattice vectors:
-1/2 0 1/2
1/2 0 1/2
0 1 0
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM3+	(a,-1.732a)	139 I4/mmm	1
GM5-	(0,0,a)	121 I-42m	1
X3+	(a,0,0)	128 P4/mnc	2
X2-	(a,0,0)	137 P4_2/nmc	2

Coupled OP.

KANGUB01

Parent: 141 D4h-19, I4_1/amd, I4_1/a2/m2/d, origin choice 2
Subgroup: 88 C4h-6, I4_1/a, I4_1/a, origin choice 2
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 1/2 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	141 I4_1/amd	1
GM3+	(a)	88 I4_1/a	1

GM3+ is the primary OP.

(methane III)

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 64 D2h-18, Cmca, C2/m2/c2_1/a
Lattice vectors:
2 0 0
0 1 1
0 -1 1
origin: 1/2 0 0

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	225 Fm-3m	1
GM3+		(a,1.732a)	139 I4/mmm	1
GM5+		(0,a,0)	71 Immm	1
SM2	1/4	(0,0,0,0,0,0,0,0,0,0,a,0)	51 Pmma	4
L1-		(a,0,a,0)	67 Cmma	4
L3-		(a,0.268a,0,0,a,0.268a,0,0)	67 Cmma	4
X1+		(0,0,a)	123 P4/mmm	2
X4+		(0,0,a)	131 P4_2/mmc	2
W2		(a,0,0,0,0,0)	139 I4/mmm	4
W3		(0,a,0,0,0,0)	140 I4/mcm	4

Coupled OP.

YIMWEW

Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup: 60 D2h-14, Pbcn, P2_1/b2/c2_1/n
Lattice vectors:
0 3 0
-1 0 1
1 0 1
origin: -1/2 0 0

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	229 Im-3m	1
GM3+		(a,-1.732a)	139 I4/mmm	1
GM5+		(0,0,a)	69 Fmmm	1

DT5	5/6	(a,-a,a,a,0,0,0,0,0,0,0,0)	64	Cmca	6
DT1	1/3	(a,0,0,0,0,0)	139	I4/mmm	3
DT3	1/3	(0,a,0,0,0,0)	69	Fmmm	3
H4+		(a,-a,0)	64	Cmca	2
H5+		(a,a,0)	64	Cmca	2
N1-		(0,0,a,0,0,0)	68	Ccca	2
N4-		(0,0,a,0,0,0)	63	Cmcm	2
D2	1/6	(0,0,a,0,0,0,0,0,0,0,0,0)	68	Ccca	6
D3	1/6	(0,0,0,0,0,0,0,0,0,a,0,0)	63	Cmcm	6

Coupled OP.

RASDOE & TFMETH02

Parent: 70 D2h-24, Fddd, F2/d2/d2/d, origin choice 2
Subgroup: 15 C2h-6, C2/c, C12/c1, unique axis b, cell choice 1
Lattice vectors:
0 -1 0
-1 0 0
0 1/2 -1/2
origin: 1/4 0 1/4

Irrep	Dir	Subgroup	Size
GM1+	(a)	70 Fddd	1
GM3+	(a)	15 C2/c	1

GM3+ is the primary OP.

REKYUB

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 15 C2h-6, C2/c, C12/c1, unique axis b, cell choice 1
Lattice vectors:
-1/2 1 -1/2
-1/2 0 1/2
1 0 1
origin: -1/4 0 -1/4

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM3+	(a,-1.732a)	139 I4/mmm	1
GM4+	(a,0,-a)	12 C2/m	1
GM5+	(a,a,b)	12 C2/m	1
L1-	(a,0,0,0)	167 R-3c	2
L3-	(a,3.732a,0,0,0,0,0,0)	15 C2/c	2

L3- is the primary OP.

MECKOU

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 12 C2h-3, C2/m, C12/m1, unique axis b, cell choice 1
Lattice vectors:
1/2 -1/2 -1
1/2 1/2 0
1/2 -1/2 1
origin: -1/4 1/4 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM3+	(a,0)	139 I4/mmm	1
GM4+	(a,a,0)	12 C2/m	1
GM5+	(a,b,-b)	12 C2/m	1
L2-	(0,0,0,a)	166 R-3m	2
L3-	(0,0,0,0,0,0,a,a)	12 C2/m	2

L3- is the primary OP.

MECKUA

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 14 C2h-5, P2_1/c, P12_1/c1, unique axis b, cell choice 1
Lattice vectors:
1/2 1 -1/2

1/2 0 1/2
1 0 -1
origin: -1/2 -1/4 1/4

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM3+	(a,-1.732a)	139 I4/mmm	1
GM4+	(a,0,a)	12 C2/m	1
GM5+	(a,-a,b)	12 C2/m	1
L2+	(0,a,0,0)	167 R-3c	2
L3+	(0,0,a,3.732a,0,0,0,0)	15 C2/c	2
L1-	(0,0,a,0)	167 R-3c	2
L3-	(0,0,0,0,a,3.732a,0,0)	15 C2/c	2
X2-	(a,0,0)	137 P4_2/nmc	2
X3-	(a,0,0)	129 P4/nmm	2
X5-	(a,0,0,0,0,0)	59 Pmmn	2

Coupled OP.

TOHSUE

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 14 C2h-5, P2_1/c, P12_1/c1, unique axis b, cell choice 1
Lattice vectors:
-1/2 0 1/2
1/2 0 1/2
0 2 0
origin: 0 -1/4 -1/4

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	225 Fm-3m	1
GM3+		(a,-1.732a)	139 I4/mmm	1
GM4+		(a,0,a)	12 C2/m	1
GM5+		(a,-a,b)	12 C2/m	1
DT2	3/4	(a,-a,0,0,0,0)	138 P4_2/ncm	4
DT4	3/4	(a,a,0,0,0,0)	130 P4/ncc	4
DT5	3/4	(0,a,-a,0,0,0,0,0,0,0,0,0)	62 Pnma	4
X2-		(a,0,0)	137 P4_2/nmc	2
X3-		(a,0,0)	129 P4/nmm	2
X5-		(a,0,0,0,0,0)	59 Pmmn	2

Coupled OP.

CARBTC07 & CTBROM

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 15 C2h-6, C2/c, C12/c1, unique axis b, cell choice 1
Lattice vectors:
-2 -1 -1
0 1 -1
2 -1 -1
origin: -1/2 1/2 1/2

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	225 Fm-3m	1
GM3+		(a,1.732a)	139 I4/mmm	1
GM4+		(0,a,-a)	12 C2/m	1
GM5+		(a,b,a)	12 C2/m	1
LD2	3/4	(0,a,0,0,0,-a,0,0)	167 R-3c	4
LD3	3/4	(0,0,a,0.268a,0,0,0,0,0,0,0.268a,a,0,0,0,0)	15 C2/c	4
L1-		(0,a,0,a)	67 Cmma	4
L2-		(a,b,c,-b)	12 C2/m	8
L3-		(a,-3.732a,b,c,d,-3.732d,0.866b+0.500c,0.500b-0.866c)	12 C2/m	8
X1+		(a,-a,b)	123 P4/mmm	4
X2+		(a,a,0)	123 P4/mmm	4
X3+		(a,a,0)	134 P4_2/nnm	4
X4+		(a,-a,b)	134 P4_2/nnm	4
X5+		(a,b,-b,a,0,c)	12 C2/m	4
C1	1/2,1/4	(0,0,a,0,0,0,0,a,0,0,0,0,0,0,a,0,0,0,0,a,0,0,0,0)	12 C2/m	8
C2	1/2,1/4	(0,0,a,0,0,0,0,-a,b,0,0,0,0,0,-a,0,0,0,0,a,-b,0,0,0)	15 C2/c	16

C2 is the primary OP.

MEZDIE01 & MEZDOK01

Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup: 2 Ci-1, P-1, P-1
Lattice vectors:
1/2 1/2 1/2
1 0 -1
-1/2 1/2 -1/2
origin: -1/4 -1/4 1/4

Irrep	Dir	Subgroup	Size
GM1+	(a)	229 Im-3m	1
GM2+	(a)	204 Im-3	1
GM3+	(a,b)	71 Immm	1
GM4+	(a,b,c)	2 P-1	1
GM5+	(a,b,c)	2 P-1	1
N1-	(0,0,a,0,0,0)	68 Ccca	2
N2-	(0,0,0,a,0,0)	63 Cmcm	2
N3-	(0,0,a,0,0,0)	67 Cmma	2
N4-	(0,0,0,a,0,0)	63 Cmcm	2

Coupled OP.

OHABEE

Parent: 229 Oh-9, Im-3m, I4/m-32/m
Subgroup: 2 Ci-1, P-1, P-1
Lattice vectors:
1/2 1/2 1/2
1 -1 0
1 1 -2
origin: -1 -1/2 1

Irrep	k params	Dir	Subgroup	Size
GM1+		(a)	229 Im-3m	1
GM2+		(a)	204 Im-3	1
GM3+		(a,b)	71 Immm	1
GM4+		(a,b,c)	2 P-1	1
GM5+		(a,b,c)	2 P-1	1
LD1	1/3	(a,0,0,0,-1.732a,0,0,0)	164 P-3m1	3
LD2	1/3	(a,0,0,0,0.577a,0,0,0)	147 P-3	3
LD3	1/3	(a,b,0,0,0,0,0,0,-0.577a-1.155b,-1.155a-0.577b,0,0,0,0,0,0)	2 P-1	3
N1-		(0,0,0,0,a,0)	68 Ccca	2
N2-		(0,0,0,0,0,a)	63 Cmcm	2
N3-		(0,0,0,0,a,0)	67 Cmma	2
N4-		(0,0,0,0,0,a)	63 Cmcm	2
C1	1/6,2/3	(a,0,0,0,0,0,0,0,0,0,0,0,-0.577a,0,0,0,0,0,0,0,0,0,0,0)	11 P2_1/m	6
C2	1/6,2/3	(a,0,0,0,0,0,0,0,0,0,0,0,1.732a,0,0,0,0,0,0,0,0,0,0,0)	13 P2/c	6

Coupled OP.

Dimer Packings:

FOJBUB & VADRAU

Parent: 225 Oh-5, Fm-3m, F4/m-32/m
Subgroup: 205 Th-6, Pa-3, P2_1/a-3
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	225 Fm-3m	1
GM2+	(a)	202 Fm-3	1
X5+	(a,a,a,a,a,a)	205 Pa-3	4

X5+ is the primary OP.

LUFYEQ

Parent: 141 D4h-19, I4_1/amd, I4_1/a2/m2/d, origin choice 2
Subgroup: 88 C4h-6, I4_1/a, I4_1/a, origin choice 2
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 1/2 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	141 I4_1/amd	1
GM3+	(a)	88 I4_1/a	1

GM3+ is the primary OP.

CARBTC

Parent: 166 D3d-5, R-3m, R-32/m, hexangonal axes
Subgroup: 14 C2h-5, P2_1/c, P12_1/c1, unique axis b, cell choice 1
Lattice vectors:
-2/3 -1/3 -1/3
0 1 0
2 1 0
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	166 R-3m	1
GM3+	(a,0)	12 C2/m	1
F2+	(0,a,0)	14 P2_1/c	2

F2+ is the primary OP.

Mixed

KOXKOX, RUQMEV, & SENLAY

Parent: 223 Oh-3, Pm-3n, P4_2/m-32/n
Subgroup: 218 Td-4, P-43n, P-43n
Lattice vectors:
1 0 0
0 1 0
0 0 1
origin: 0 0 0

Irrep	Dir	Subgroup	Size
GM1+	(a)	223 Pm-3n	1
GM2-	(a)	218 P-43n	1

GM2- is the primary OP.

Richard B. McClurg, April, 2008

Table 9. Identifiers, chemical formulas, and assigned frameworks of the tetrahedral data set. The adamantane and cubane molecular frameworks are substituted derivatives of these molecules, while MX_4 molecules have a central atom (denoted M) with four identical X groups.

Identifier	formula	framework
ADAMAN08	C10 H16	adamantane
BASXOI	C4 H12 Se6 Sn4	adamantane
BOGMEP	C24 H48 Cl6 Cu4 N16 O1	other
CAMPOV	C16 H36 N4 Sn4	cubane
CANFIG	C4 H24 B4 U1	MX_4
CANFOM	C4 H24 B4 Th1	MX_4
CARBTC	C1 Cl4	MX_4
CARBTC07	C1 Cl4	MX_4
CTBROM	C1 Br4	MX_4
CUCZUV	C20 H36	tetrahedrane
DEQPAQ	C36 H100 B4 N12 Na4	other
DILWIE01	C16 H48 Pt4 S4	cubane
DOCNIS	C8 H12 S6	adamantane
FOHCUA	C12 Ni4 O18 P4	adamantane
FOJBUB02	C4 Ni1 O4	MX_4
FUZLUH	C12 Co4 O12 Sb4	cubane
FUZTEZ	H16 B4 Np1	MX_4
FUZVOL	H16 B4 Hf1	MX_4
GERHOA	C4 H12 Cl12 N4 Sb4	cubane
GUTCED	C26 H32	other
HMGETP	C12 H36 Ge6 P4	adamantane
HMSIPA	C12 H36 P4 Si6	adamantane
HXMTAM07	C6 H12 N4	adamantane
JEYSEL	C18 H36 Ni4 O6 P4	tetrahedrane
JUFWUC	C12 H40 Cs4 N4 Si4	cubane
KANGUB01	C10 H12 I4	adamantane
KELREY	C12 H36 Cl4 Ti4	cubane
KOXKOX	C16 H36 Ga4 Se4	cubane
KUJSIR	C20 H48 O4 Zn4	cubane
LUFYEQ	C12 H12 Si1	MX_4
MECKIO	C16 H36 Cl4 In4 N4	cubane
MECKOU	C16 H36 Br4 In4 N4	cubane
MECKUA	C16 H36 I4 In4 N4	cubane
MESIAD	C12 H36 As4 Si6	adamantane
MEZDIE01	C12 H36 Si1 Sn4	MX_4
MEZDOK01	C12 H36 Ge1 Sn4	MX_4
MPTHOT01	C12 H40 O4 Pt4	cubane
MSISUL10	C4 H12 S6 Si4	adamantane
MTRETC10	C16 H12 O12 Re4 S4	cubane
MXSNOX	C4 H12 O8 Sn6	other
MZNMOX10	C8 H24 O4 Zn4	cubane
NIWMIP	C12 H36 Al4 N4 S6	adamantane
OHABEE	C16 H36 Si4	tetrahedrane
POSLOY10	C12 Cl4 O12 Tc4	cubane
QUGBOJ	C16 O16 Rh6	other
RASDOE	C16 H48 Ga4 N4 Si4	cubane
REKYUB	C16 H36 Ga4 S4	cubane
RIMMOP	C16 H40 Al4 N4	cubane
RIMNAC	C20 H48 Al4 N4	cubane
RUQMEV	C12 H36 Cu4 I4 N4	cubane
SENLAY	C16 H36 P4 Si4	cubane
TCYMET	C5 N4	MX_4
TFMETH02	C1 F4	MX_4
TMEPTC	C12 H36 Cl4 Pt4	cubane
TMGEHS10	C4 H12 Ge4 S6	adamantane
TMSIAD	C10 H24 Si4	adamantane
TMSNHS10	C4 H12 S6 Sn4	adamantane
TOHSUE	C16 F12 O12 P4 Ru4	cubane
VADRAU	C4 H12 Pb1	MX_4
VAFWAA	C12 Bi4 Co4 O12	cubane
VAVYAS	C20 H36 P4	cubane
XAGXAE	P4 S10	adamantane
XUWROW	C20 H48 Mg4 O4	cubane
YEMRIR	O6 P4 S4	adamantane
YEYQAU	C12 O12 Ru4 Se4	cubane
YIMWEW	C10 H16 O4	adamantane
ZEYHIU	C20 H48 Cd4 O4	cubane
ZIZHIZ	C12 H4 Mn4 O16	cubane
ZNOXAC01	C12 H18 O13 Zn4	other
ZZZKDW01	C1 I4	MX_4