LETTERS

Dense packings of the Platonic and Archimedean solids

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Dense particle packings have served as useful models of the structures of liquid, glassy and crystalline states of matter[1–4], granular media[3,5], heterogeneous materials[3] and biological systems[6–8]. Probing the symmetries and other mathematical properties of the densest packings is a problem of interest in discrete geometry and number theory[9–11]. Previous work has focused mainly on spherical particles—very little is known about dense polyhedral packings. Here we formulate the generation of dense packings of polyhedra as an optimization problem, using an adaptive fundamental cell subject to periodic boundary conditions (we term this the 'adaptive shrinking cell' scheme). Using a variety of multi-particle initial configurations, we find the densest known packings of the four non-tiling Platonic solids (the tetrahedron, octahedron, dodecahedron and icosahedron) in three-dimensional Euclidean space. The densities are 0.782..., 0.947..., 0.904... and 0.836..., respectively. Unlike the densest tetrahedral packing, which must not be a Bravais lattice packing, the densest packings of the other non-tiling Platonic solids that we obtain are their previously known optimal (Bravais) lattice packings. Combining our simulation results with derived rigorous upper bounds and theoretical arguments leads us to the conjecture that the densest packings of the Platonic and Archimedean solids with central symmetry are given by their corresponding densest lattice packings. This is the analogue of Kepler's sphere conjecture for these solids.

A large collection of non-overlapping solid objects (particles) in d-dimensional Euclidean space $\mathbb{R}^d$ is called a packing. The packing density ϕ is defined as the fraction of space $\mathbb{R}^d$ covered by the particles. A problem that has been a source of fascination to mathematicians and scientists for centuries is the determination of the densest arrangement(s) of particles that do not tile space and the associated maximal density $\phi_{\max}$ (ref. 9). Most previous work has focused on spherical particles, but even for this simple shape the problem is notoriously difficult. Indeed, Kepler's conjecture concerning the densest sphere packing arrangement was only proved by Hales in 2005 (ref. 10).

Attention has very recently turned to finding the maximum-density packings of nonspherical particles in $\mathbb{R}^3$, including ellipsoids[12], tetrahedra[13,14], and superballs[15]. Very little is known about the densest packings of polyhedral particles that do not tile space, including the majority of the Platonic and Archimedean solids studied by the ancient Greeks. The difficulty in obtaining dense packings of polyhedra is related to their complex rotational degrees of freedom and to the non-smooth nature of their shapes.

The Platonic solids (mentioned in Plato's *Timaeus*) are convex polyhedra with faces composed of congruent convex regular polygons. There are exactly five such solids: the tetrahedron, icosahedron, dodecahedron, octahedron and cube (see Fig. 1). An Archimedean solid is a highly symmetric, semi-regular convex polyhedron composed of two or more types of regular polygons meeting in identical vertices. There are thirteen Archimedean solids (see Fig. 1). We note that the tetrahedron (P1) and truncated tetrahedron (A1) are the only Platonic and Archimedean solids, respectively, that are not centrally symmetric. A particle is centrally symmetric if it has a centre C that bisects every chord through C connecting any two boundary points of the particle. We will see that this type of symmetry is fundamental in determining the nature of the dense packing arrangements.

Some definitions are in order here. A lattice Λ in $\mathbb{R}^3$ is an infinite set of points generated by a set of discrete translation operations (defined by integer linear combinations of a basis of $\mathbb{R}^3$) (ref. 4). A (Bravais) lattice packing is one in which the centroids of the non-overlapping particles are located at the points of Λ, each oriented in the same direction. The space $\mathbb{R}^3$ can then be geometrically divided into identical regions F called fundamental cells, each of which contains just the centroid of one particle. Thus, the density of a lattice packing is given by

$$\phi = \frac{v_{\text{particle}}}{V_{\text{F}}} \tag{1}$$

where v_{particle} is the volume of a particle and V_{F} is the volume of a fundamental cell. A periodic packing of particles is obtained by placing a fixed non-overlapping configuration of N particles (where $N \geq 1$) with arbitrary orientations in each fundamental cell of a lattice Λ. Thus, the packing is still periodic under translations by Λ, but the N particles can occur anywhere in the chosen cell subject to the non-overlap condition. The density of a periodic packing is given by

$$\phi = \frac{N v_{\text{particle}}}{V_{\text{F}}} \tag{2}$$

We formulate the problem of generating dense packings of non-overlapping polyhedra within an adaptive fundamental cell subject to periodic boundary conditions as an optimization problem (see Methods Summary). We call this optimization scheme the 'adaptive shrinking cell' (ASC). Figure 2 illustrates a simple sequence of configuration changes for a four-particle packing.

Finding the densest packings of regular tetrahedra is part of the eighteenth problem in Hilbert's famous set of problems. The densest (Bravais) lattice packing of tetrahedra (which requires all of the tetrahedra to have the same orientations) has the relatively low density $\phi_{\max}^{\text{lattice}} = 18/49 = 0.367\ldots$ and each tetrahedron touches 14 others[16]. Recently, Conway and Torquato showed that the densest packings of tetrahedra must not be Bravais lattice packings, and found packings with density as large as $\phi \approx 0.72$ (ref. 13). P. Chaikin, S. Wang and A. Jaoshvili experimentally generated jammed disordered packings of nearly tetrahedral dice with $\phi \approx 0.75$ (unpublished work). Chen[14] has recently discovered a periodic packing of tetrahedra with $\phi = 0.7786\ldots$, which we call the 'wagon-wheels' packing because the basic subunits consist of

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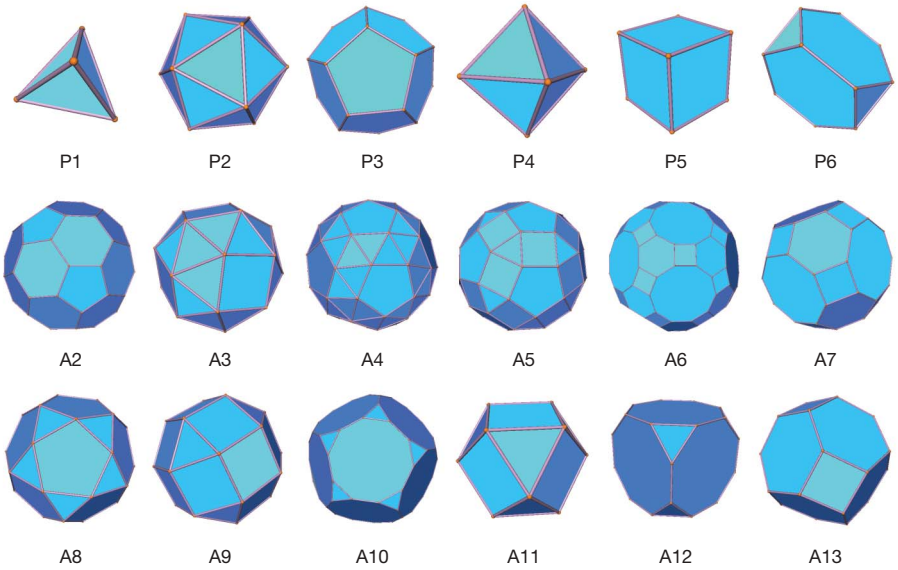

Figure 1 | The five Platonic solids and the 13 Archimedean solids. The five Platonic solids are the tetrahedron (P1), icosahedron (P2), dodecahedron (P3), octahedron (P4) and cube (P5). The 13 Archimedean solids are the truncated tetrahedron (A1), truncated icosahedron (A2), snub cube (A3), snub dodecahedron (A4), rhombicosidodecahedron (A5), truncated icosidodecahedron (A6), truncated cuboctahedron (A7), icosidodecahedron (A8), rhombicuboctahedron (A9), truncated dodecahedron (A10), cuboctahedron (A11), truncated cube (A12), and truncated octahedron (A13). The cube (P5) and truncated octahedron (A13) are the only Platonic and Archimedean solids, respectively, that tile space.

two orthogonally intersecting 'wagon wheels'. A wagon wheel consists of five contacting tetrahedra packed around a common edge (see figure 1a of ref. 13).

We begin by solving the ASC scheme to obtain dense packings of tetrahedra using initial configurations based upon low-density versions of the aforementioned packings. Initial conditions based on periodic copies of the wagon-wheels packing with 72 particles per cell lead to the densest packing of tetrahedra reported to date with $\phi = 0.782021\ldots$ (see Fig. 3). Its lattice vectors and other characteristics are given in the Supplementary Information. The preference for face-to-face (not vertex-to-face) contacts and the lack of central symmetry ensure that dense tetrahedral packings must be non-lattice structures.

To obtain dense packings of icosahedra, dodecahedra and octahedra, we use a wide range of initial configurations. These include multi-particle configurations (with N ranging from 20 to 343) of random 'dilute' packings and a variety of lattice packings with a wide range of densities. For icosahedra, dodecahedra and octahedra, we obtain final packings with densities at least as large as $0.836315\ldots$, $0.904002\ldots$ and $0.947003\ldots$, respectively, which are extremely close in structure and density to their corresponding optimal lattice packings with $\phi_{\max}^{\text{lattice}} = 0.836357\ldots$ (ref. 17), $\phi_{\max}^{\text{lattice}} = \left(5+\sqrt{5}\right)/8 = 0.904508\ldots$ (ref. 17) and $\phi_{\max}^{\text{lattice}} = 18/19 = 0.947368\ldots$ (ref. 18), respectively. Figure 3 shows the optimal lattice packings of icosahedra, dodecahedra and octahedra, in which each particle contacts 12, 12 and 14 others, respectively. Our simulation results strongly suggest that the optimal lattice packings of the centrally symmetric Platonic solids are indeed the densest packings of these particles, especially since these arise from a variety of initial dilute multi-particle configurations within an adaptive fundamental cell.

We can show that the maximal density $\phi_{\max}$ of a packing of congruent nonspherical particles of volume v_{particle} is bounded from above according to:

$$\phi_{\max} \leq \phi_{\max}^{\text{upper bound}} = \min\left[\frac{v_{\text{particle}}}{v_{\text{sphere}}}\frac{\pi}{\sqrt{18}},\ 1\right] \qquad (3)$$

where v_{sphere} is the volume of the largest sphere that can be inscribed in the nonspherical particle and $\pi/\sqrt{18}$ is the maximal sphere-packing density. The proof is given in the Supplementary Information. The upper bound (3) will be relatively tight for packings of nonspherical particles provided that the asphericity γ (equal to the ratio of the circumradius to the inradius, see online-only Methods) of the particle

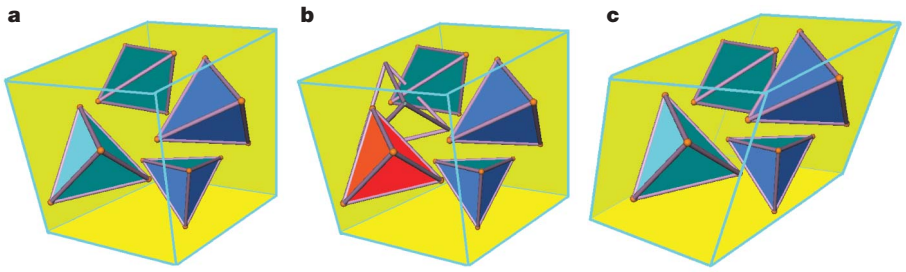

Figure 2 | Sequential changes of a four-particle packing configuration according to the design variables in the ASC algorithm. By efficiently exploring the design-variable space, which consists of the particle configurational space and the space of lattices (owing to our use of an adaptive fundamental cell), the ASC scheme enables us to find a point in the design-variable space in the neighbourhood of the starting point that has a higher packing density than the initial density. The process is continued until the deepest minimum of the objective function (a maximum of packing density) is obtained, which could be either a local or global optimum. Here we show such a sequence. **a**, An initial configuration of four particles. **b**, A trial move of a randomly selected particle (red) that is rejected because it overlaps another particle. This is determined precisely using the separation axis theorem[26]. **c**, A trial move that is accepted, which results in a deformation and compression (small in magnitude) changing the fundamental cell shape and size as well as the relative distances between the particles.

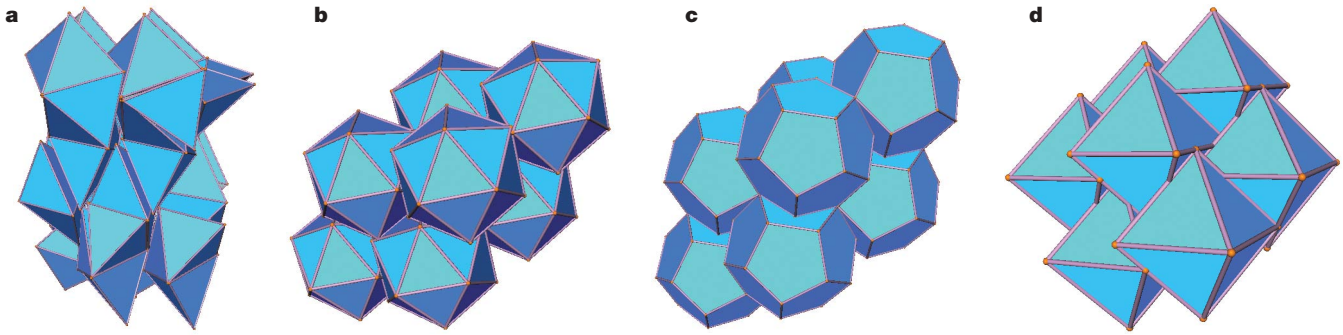

Figure 3 | Portions of the densest packing of tetrahedra obtained from our simulations, and the optimal lattice packings of the icosahedra, dodecahedra and octahedra to which our simulations converge. All of these packings are at least locally jammed, that is, each particle cannot be translated or rotated while fixing the positions and orientations of all the other particles[27,28]. We emphasize that even though the latter three cases begin with complex multi-particle initial configurations in the large fundamental (repeating) cell, they all converge to packings in which a smaller repeat unit contains only one centroid, that is, they all converge to Bravais lattice packings and, in fact, the corresponding densest lattice packings. **a**, Tetrahedral packing. We depict the 72 particles in the fundamental cell of this non-lattice packing. Within the cell, the particles are characterized by short-range translational order and a preference for face-to-face contacts (see Supplementary Information). **b**, Optimal lattice packing of icosahedra. **c**, Optimal lattice packing of dodecahedra. **d**, Optimal lattice packing of octahedra.

is not large. Bound (3) cannot generally be sharp (that is, exact) for a nontiling, nonspherical particle, so any packing whose density is close to the upper bound (3) is nearly optimal, if not optimal.

Figure 4 compares the density of the densest lattice packings of the Platonic and Archimedean solids to the corresponding upper bounds on the maximal density for such packings. The central symmetry of the majority of the Platonic and Archimedean solids and their associated relatively small asphericities explain the corresponding small differences between $\phi_{\max}^{\text{lattice}}$ and $\phi_{\max}^{\text{upper bound}}$ and is consistent with our simulation findings that strongly indicate that their optimal arrangements are their respective densest lattice packings.

Why should the densest packings of the centrally symmetric solids be their corresponding optimal lattice packings? First, face-to-face contacts allow such polyhedral packings to achieve higher densities because they enable the contacting centroids around each particle to come closer together. Second, face-to-face contacts are maximized when each particle has the same orientation because of the central symmetry and the equivalence of the three principal axes (associated with the small asphericity) of the solid. This is consistent with a lattice packing, the densest of which is the optimal one. These arguments in conjunction with our simulation results for the Platonic solids and rigorous bounds lead us to the following conjecture: The densest packings of the centrally symmetric Platonic and Archimedean solids are given by their corresponding optimal lattice packings. This is the analogue of Kepler's sphere conjecture for these solids.

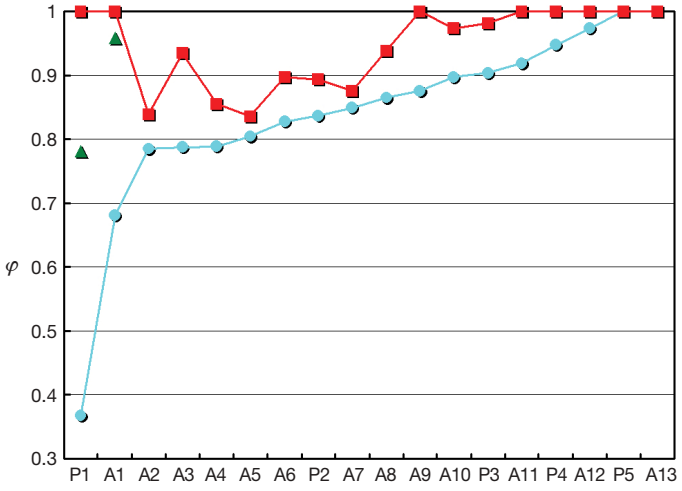

Figure 4 | Comparison of the densest known lattice packings (blue circles) of the Platonic and Archimedean solids[16–18] to the corresponding upper bounds (red squares) obtained from bound (3). The large asphericity and lack of central symmetry of the tetrahedron (P1) and truncated tetrahedron (A1) are consistent with the large gaps between their upper-bound densities and densest-lattice-packing densities, and the fact that there are non-lattice packings with densities appreciably greater than $\phi_{\max}^{\text{lattice}}$ (green triangles). The truncated tetrahedron is the only non-centrally symmetric Archimedean solid, the densest known packing of which is a non-lattice packing with two particles per fundamental cell and a density at least as high as 23/24 = 0.958333… (ref. 13).

There is no reason to believe that denser packings of tetrahedra cannot be achieved by using even better initial conditions than those based on the wagon-wheels packing and a larger number of particles. We observe that the densest packings of all of the Platonic and Archimedean solids reported here as well as the densest known packings of superballs[15] and ellipsoids[12] have densities that exceed the optimal sphere packing density $\phi_{\max}^{\text{sphere}} = \pi/\sqrt{18} = 0.7408\ldots$. These results are consistent with Ulam's conjecture[19], which may be violated if the convex particle has little or no symmetry, but a counterexample has yet to be given.

How does our conjecture extend to other polyhedral packings? It is natural to group the infinite families of prisms and antiprisms[20] with the Archimedean solids. A prism is a polyhedron having bases that are parallel, congruent polygons and sides that are parallelograms. An antiprism is a polyhedron having bases that are parallel, congruent polygons and sides that are alternating bands of triangles. Prisms with an even number of sides and antiprisms are centrally symmetric and so it may be that Bravais lattices of such solids are optimal. However, prisms with an odd number of sides are not centrally symmetric and thus their optimal packings may not be Bravais lattices. In future work, we will determine whether our conjecture extends to prisms and antiprisms.

METHODS SUMMARY

The objective function in our ASC optimization scheme is taken to be the negative of the packing density ϕ. Starting from an initial packing configuration in the fundamental cell, the positions and orientations of the polyhedra are design variables for the optimization. Importantly, we also allow the boundary of the fundamental cell to deform as well as shrink or expand such that there is a net shrinkage (increase of the density) in the final state. Thus, the deformation and compression/expansion of the cell boundary are also design variables. We are not aware of any packing algorithm that employs both a sequential search of the configurational space of the particles and the space of lattices via an adaptive fundamental cell that shrinks on average to obtain dense packings. The ASC has a number of novel features that distinguish it from previous packing algorithms that have been devised for spheres[21–23], ellipsoids[24,25] and superballs[15] (see online-only Methods for details).

Full Methods and any associated references are available in the online version of the paper at www.nature.com/nature.

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Supplementary Information is linked to the online version of the paper at www.nature.com/nature.

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Author Contributions S.T. devised the algorithm and upper bounds, performed theoretical analysis, and wrote the paper. Y.J. implemented the algorithm, performed theoretical analysis, commented on the manuscript and created all of the figures.

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METHODS

The ASC optimization problem could be solved using various techniques, depending on the shapes of the particles. For example, for spheres, we have shown that linear programming techniques can efficiently produce optimal solutions (unpublished work). However, for polyhedra, the complex non-overlap conditions make the ASC scheme inefficient to solve using linear programming methods. For polyhedral particles, we solve the ASC optimization problem using a standard Monte Carlo procedure with a Metropolis acceptance rule for trial moves to search the design-variable space efficiently, which contains both the configuration space of the particles and the space of lattices.

In our implementation, a polyhedral particle is represented by the position of its centroids as well as the coordinates of all its vertices relative to the centroid. Although this representation contains redundant information, it is a convenient way to deal with the rotational motions of the polyhedra. To search the configuration space of the particles, small random trial moves of arbitrarily selected particles are attempted sequentially for each particle. Each trial move is equally likely to be a translation of the centroid of the particle or a rotation of the particle about a randomly oriented axis through its centroid.

The space of lattices is searched by deforming/compressing/expanding the fundamental cell, which is completely characterized by a strain tensor in the linear regime (that is, small strain limit). The trace of the strain tensor determines the volume change of the fundamental cell and is involved in the objective function. The off-diagonal components of the tensor determine the shape change of the cell. The positions of the particles centroids are relative coordinates with respect to the lattice vectors. When the strain tensor is applied to the lattice vectors, although the relative coordinates of the centroids remain the same, the Euclidean distances between the particles will change. Thus, the deformation/compression/expansion of the fundamental cell at least in part allows for collective particle motions, which is more efficient for finding a direction in the design-variable space leading to a higher packing density. Moreover, it is the overall compression of the fundamental cell that causes the packing density to increase, not the growth of the particles, as in most molecular dynamics and Monte Carlo hard-particle packing algorithms[15,21–25]. It should be noted that for polyhedral particles, an algorithm that employs particle growth with an adaptive non-shrinking fundamental cell is computationally less efficient than the ASC scheme, which fixes the particle size while allowing the cell to shrink on average. Whereas a 'growth' algorithm requires manipulating the coordinates of the vertices of all of the particles, our 'shrinkage' method (in which the particle sizes are kept fixed) requires only the computation of the six strain components.

In the simulation, starting from an initial configuration of polyhedral particles, a trial configuration can be generated by moving (translating and rotating) a randomly chosen particle or by a random deformation and compression/expansion of the fundamental cell. If this causes interparticle overlaps, the trial configuration is rejected; otherwise, if the fundamental cell shrinks in size (which makes the density ϕ higher), the trial configuration is accepted. On the other hand, if the cell expands in size, the trial configuration is accepted with a specified probability p_{acc}, which is made to decrease as ϕ increases and approaches zero at the jamming limit[27] (that is, locally maximally dense packing) is reached. In particular, we find p_{acc}, with an initial value $p_{acc} \approx 0.35$ that decreases as a power law with an exponent equal to -1, works well for most systems that we studied. The ratio of the number of particle motions to the number of cell trial moves should be greater than unity (especially towards the end of the simulation), because compressing a dense packing could cause many overlaps between the particles. Depending on the initial configuration, the magnitudes of the particle motions and the strain components need to be chosen carefully to avoid the system getting stuck in some shallow local minimum.

A crucial aspect of any packing algorithm is the need to check for interparticle overlaps under attempted particle motions. Hard polyhedron particles, unlike spheres, ellipsoids and superballs, do not possess simple 'overlapping' functions. (The overlap function of a pair of strictly convex and smooth particles is a function of the positions, orientations and shapes of the two particles, whose value indicates whether the two particles overlap or not, or whether they are tangent to one another.) The separation axis theorem[26] enables us to check for interparticle overlaps for polyhedra up to the numerical precision of the machine. In particular, the theorem states that two convex polyhedra are separated in space if and only if there exists an axis, on which the projections of the vertices of the two polyhedra do not overlap. The separation axis is either perpendicular to one of the faces of the polyhedra or perpendicular to a pair of edges, one from each polyhedron. Thus, this reduces the number of axes that need to be checked from infinity to $[E(E-1)/2 + 2F]$, where E and F are the number of edges and number of faces of the polyhedra, respectively. A pre-check using the circumradius and inradius of the polyhedra dramatically speeds up the simulations, that is, two particles are guaranteed to overlap if the centroidal separation is smaller than twice the inradius and guaranteed not to overlap if the centroidal separation is larger than twice the circumradius. The circumsphere is the smallest sphere containing the particle. The insphere is the largest sphere than can be inscribed in the particle.

The cell method and near-neighbour list[24,25] are also used to improve the efficiency of the simulation, but are appropriately modified to incorporate the adaptive fundamental cell.

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In Figure 1 of this letter, in the top row 'A1' was incorrectly listed as 'P6'. The correct figure is shown below.