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Cellular Structures in Three Dimensions

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Cellular structures in three dimensions

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We review recent progress in the simulation of three-dimensional cellular structures, such as that of soap froth. The Surface Evolver has been used to investigate the effect of liquid fraction on the structure of bulk foam. The influence of surface constraints has also been explored.

1. Introduction

Wherever two phases separate and coexist, as in an emulsion, they are likely to form a cellular structure similar to that of a foam. Figure 1 shows a cell from a typical cellular structure. If one phase predominates, the result is a partitioning of space into polyhedral cells. More generally, the minority phase (the liquid in the case of a foam) occupies a significant volume fraction. In the language of foam science, we have a wet foam.

In the simplest cases the equilibrium principle is straightforward: the surface energy of the cells is to be minimized. The structure must constitute a minimum of surface energy for cells of specified volumes (assuming that their contents are incompressible). It need not be, and is generally not, the global minimum.

The study of such structures has been actively pursued over the last ten years. Many have taken as their starting point the survey undertaken by Weaire & Rivier (1984), but this was largely confined to two-dimensional cellular structures. We have now reached the point at which three-dimensional problems can be addressed.

First let us recall the rules of equilibrium stated by Plateau (1873) for the dry foam.

(*a*) The films which are the interfaces between cells have mean local curvatures, K, related to the pressures in the adjoining cells by Laplace's law:

$$\Delta p = 2\sigma K. \tag{1.1}$$

(*b*) The films meet three at a time on lines.

(*c*) The lines meet four at a time at vertices.

(*d*) The local symmetry at these lines is threefold, and the vertices are tetrahedrally symmetric (see figure 2).

These rules follow easily from arguments of surface tension, although a full proof of (*b*) and (*c*) with mathematical rigour was given only after a century (Taylor 1976).

Surprisingly, the precise relevance of these rules to wet foams (of finite liquid content) is a subject of active debate, as explained in the next section.

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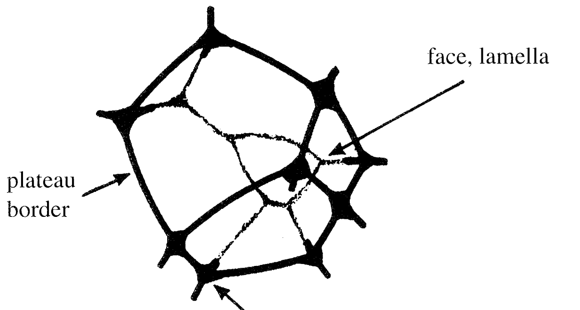

Figure 1. A single cell from a typical cellular structure.

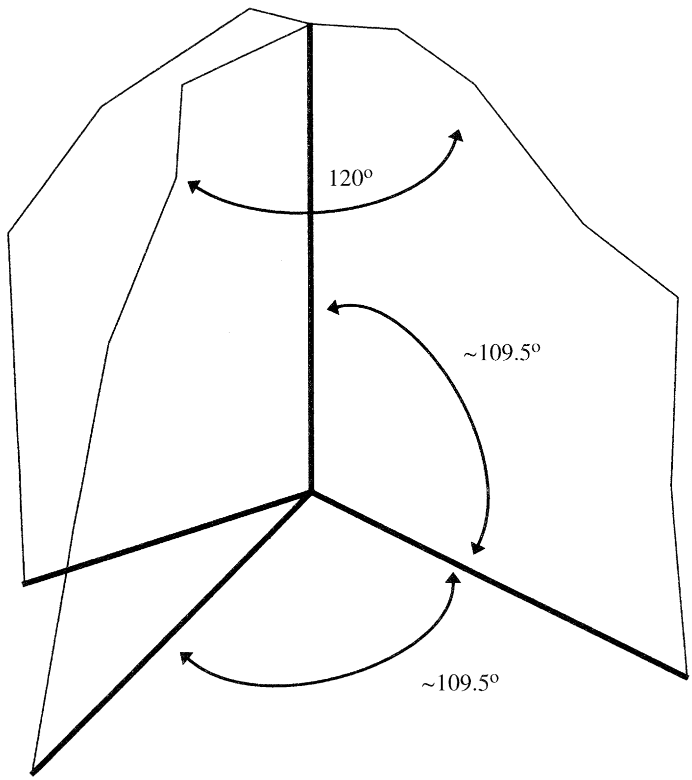

Figure 2. Illustration of Plateau's equilibrium rules.

2. The Kelvin problem

In 1994 Weaire drew attention to the following question: what is the structure of (global) minimum surface area for a foam of equal bubbles, as a function of liquid fraction?

In the dry limit we may call this the Kelvin problem, since it was first posed and analysed by Kelvin in 1887. Kelvin's proposed solution was a BCC arrangement of

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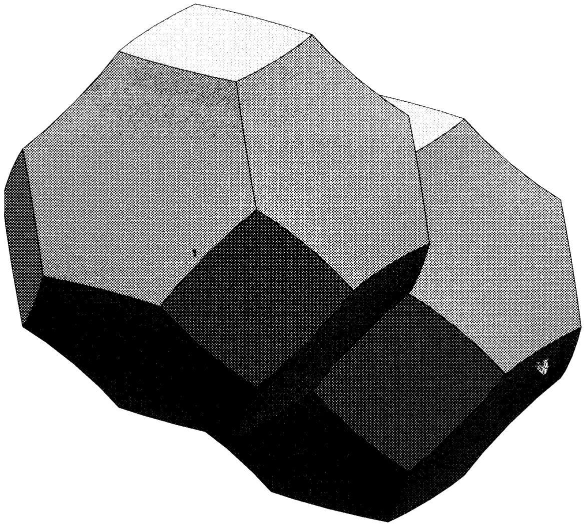

Figure 3. A cubic unit cell of Kelvin's structure consisting of two of his tetrakaidecahedra.

bubbles, the individual cell being his tetrakaidecahedron (figure 3). This is a slightly curved version of what would today be called the Wigner–Seitz cell of that structure.

The question raised in 1994 was that of the nature of the structures and structural transitions between this limit and the opposite (wet) one, at which face-centred cubic (FCC) or some other close-packing of spherical bubbles must prevail. Recall that such questions are not yet easily settled by experiment, as disorder generally prevails in practice.

In the course of investigating the problem thus posed, a largely unexpected discovery was made at an early stage (Weaire & Phelan 1994*a*). The Kelvin solution is surpassed for dry foam by another ordered structure, which is related to that of certain clathrate compounds in chemistry, or the A15 (β-tungsten) structure in metals. Figure 4*a* shows the cell centres of one periodic unit of this structure and 4*b* illustrates the structure itself. An extended region of four unit cells is shown in figure 4*c*.

Two years later, this remains the best structure yet discovered for the Kelvin problem (Sullivan & Kusner 1996). It was found using the Surface Evolver program of Brakke (1992). See figure 5 for examples of other closely related structures.

The description of wet foam structures remains of great interest and further calculations have been made on these, by use of an adapted version of the Surface Evolver (Phelan *et al.* 1995). The idealized edges and vertices of the dry foam (figure 1) are replaced by liquid regions (Plateau borders) of the form show in figure 6.

Recently, Weaire & Phelan (1996) have raised the following question. Is rule (*c*) valid for wet foam, in the dry limit? It has previously been assumed that this must be so, but it is not self-evident. Weaire & Phelan claimed to have shown that the rule was violated for one type of vertex, but it is now claimed by others that the multiple junction in question is unstable up to a very small but finite value of the liquid fraction (Brakke 1996, personal communication).

In contrast, there is a well-defined structural transition in the case of BCC (figure 8). As the liquid content is increased from zero, the quadrilateral faces shrink

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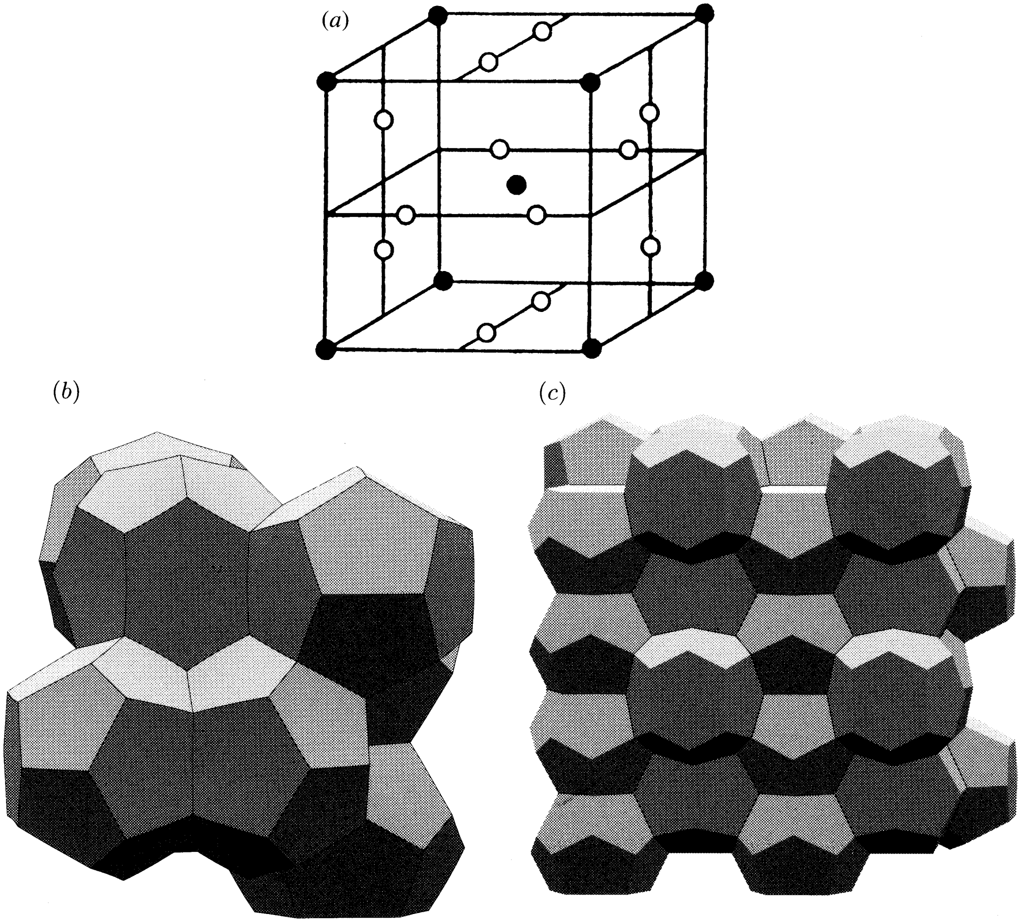

Figure 4. (*a*) The A15 (β-tungsten) structure. The atomic positions correspond to the cell centres of the structure shown in (*b*). (*b*) One unit cell of the Weaire–Phelan structure consisting of six 14-hedra and two 12-hedra. (*c*) An extended region of the same structure illustrating the stacking of the 14-hedra.

and eventually disappear at a liquid fraction of *ca.* 11%. This topological change induces an elastic instability and a structural transformation.

3. Cylindrical cellular structures

As we have said, the study of bulk ordered structures is frustrated by the failure of experimental samples to order, although it is true that small fragments of the new structure have been observed (Weaire & Phelan 1994*b*).

This difficulty is not encountered when relatively large bubbles are introduced into a cylindrical tube. Indeed any one of a remarkable variety of beautiful ordered structures can be created in a few seconds, depending on the ratio of tube to bubble diameter. They will surely provide the ideal test-bed for future experiments of many kinds. In the standard notation of the subject (Pittet *et al.* 1995), figure 9 shows the 211 and 422 cylindrical structures.

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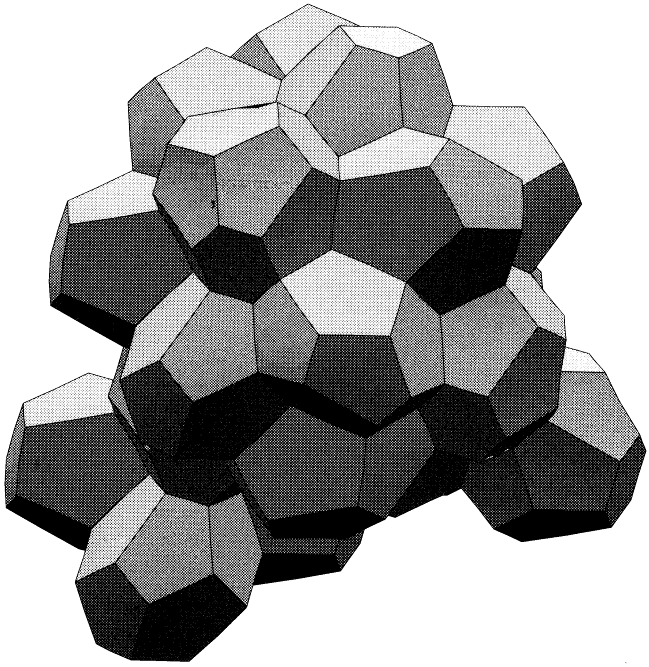
(*a*)



(*b*)

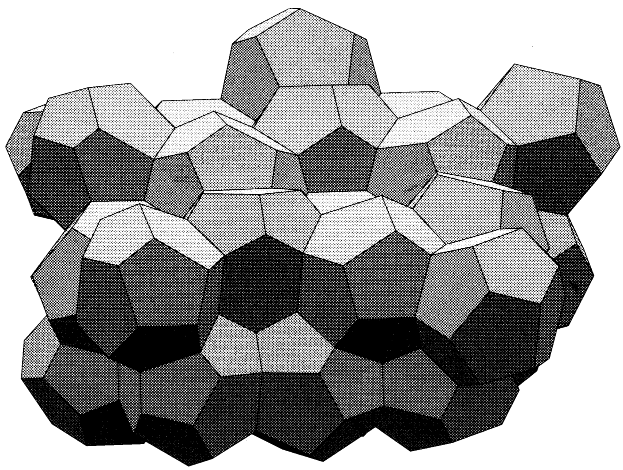


Figure 5. Other examples of possible foam structures drawn from the same class of chemical structures as A15. (*a*) C15, (*b*) σ (β-uranium).

4. Slabs and surfaces

Ordered structures also form readily at plane surfaces and in slab geometries, as discussed by Weaire & Phelan (1994*b*). Amusingly, the case of a double layer of cells between two glass plates is related to the historic debate over the bee's honeycomb (Fejes Tóth 1964; Weaire & Phelan 1994*c*). Fejes Tóth described an ideal structure (figure 10) of lower surface area than that used by the bees (figure 11). Both can

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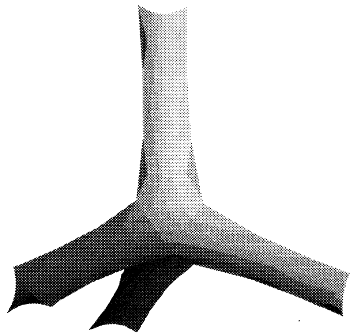

Figure 6. Detail of a single wet foam junction formed by four Plateau borders.

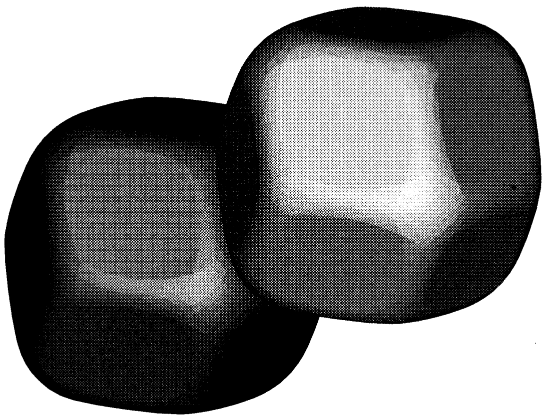

Figure 7. The cubic unit cell of the FCC wet foam structure. Note the obvious presence of eight-fold vertices.

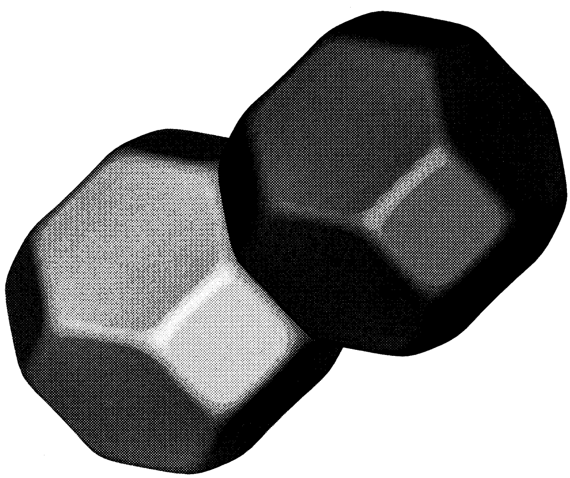

Figure 8. Kelvin's structure for a non-zero liquid fraction.

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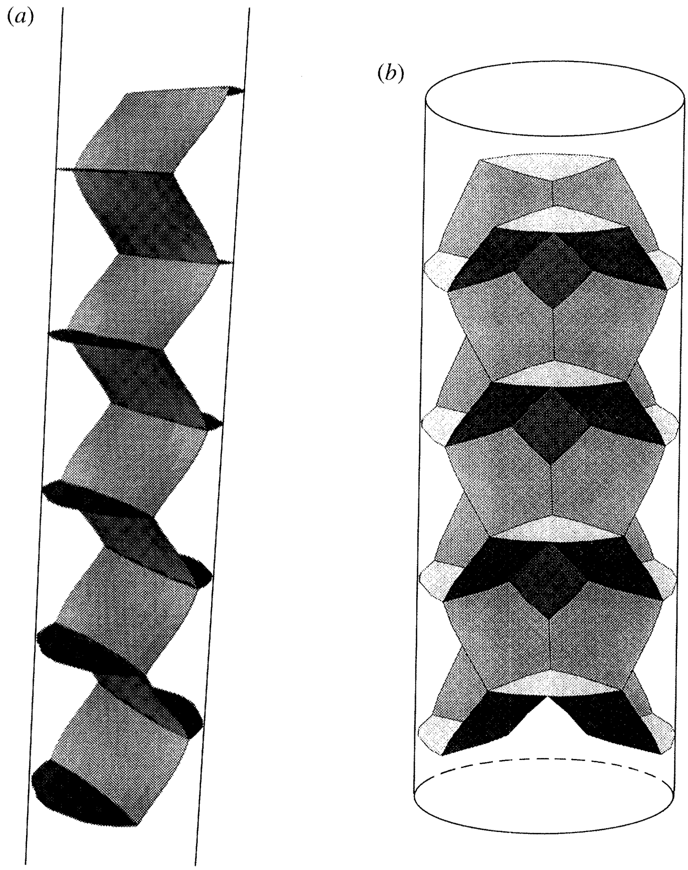

Figure 9. Two simple arrangements of foam cells in a cylinder. The (*a*) 211 and (*b*) the 422 structures.

be observed for a double layer of foam cells; Fejes Tóth's in the limit of low liquid fraction and the bee's structure in the limit of high liquid fraction.

5. Theory

What of theory, in relation to problems of global minimization? Its impotence is such that even a proof that the two-dimensional honeycomb structure is optimal (among all structures which divide the plane into equal areas) remains to be found. This makes the corresponding problem in three dimensions seem quite beyond all hope of solution. The proof in both cases is likely to be very elaborate when it comes, and heavily reliant upon computation. For the time being, and for presumably much time to come, we remain with no certain knowledge that the new structure cannot in turn be improved upon.

6. Conclusion

The rapid progress which this subject has enjoyed in the last few years is due in part to the availability of excellent software in the Surface Evolver package. It has made a significant impact on many other fields as well, ranging from abstract math-

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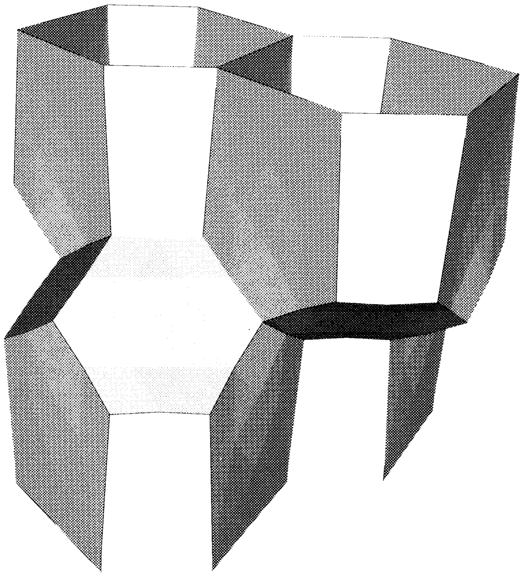
(a)



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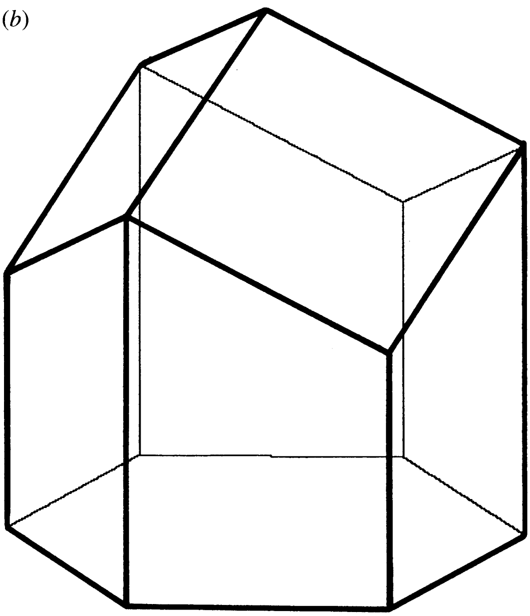

Figure 10. (a) Four Fejes Tóth cells, described by him in the context of the bee's honeycomb and also observed as a typical foam surface cell. (b) Illustration of a single bee's honeycomb cell.

ematical topology to very practical applications, such as the modelling of soldering. In addition, we now realize that in the hundred years since Kelvin played with soap films in his home, others have been too reticent to try such simple experiments. Although we have not stressed that aspect here, experimentation of a most elementary kind has guided us in many new directions. As the increasing sophistication of ex-

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perimental science runs up against the brick wall of diminished funding, such easy experiments may have a broader appeal in future.

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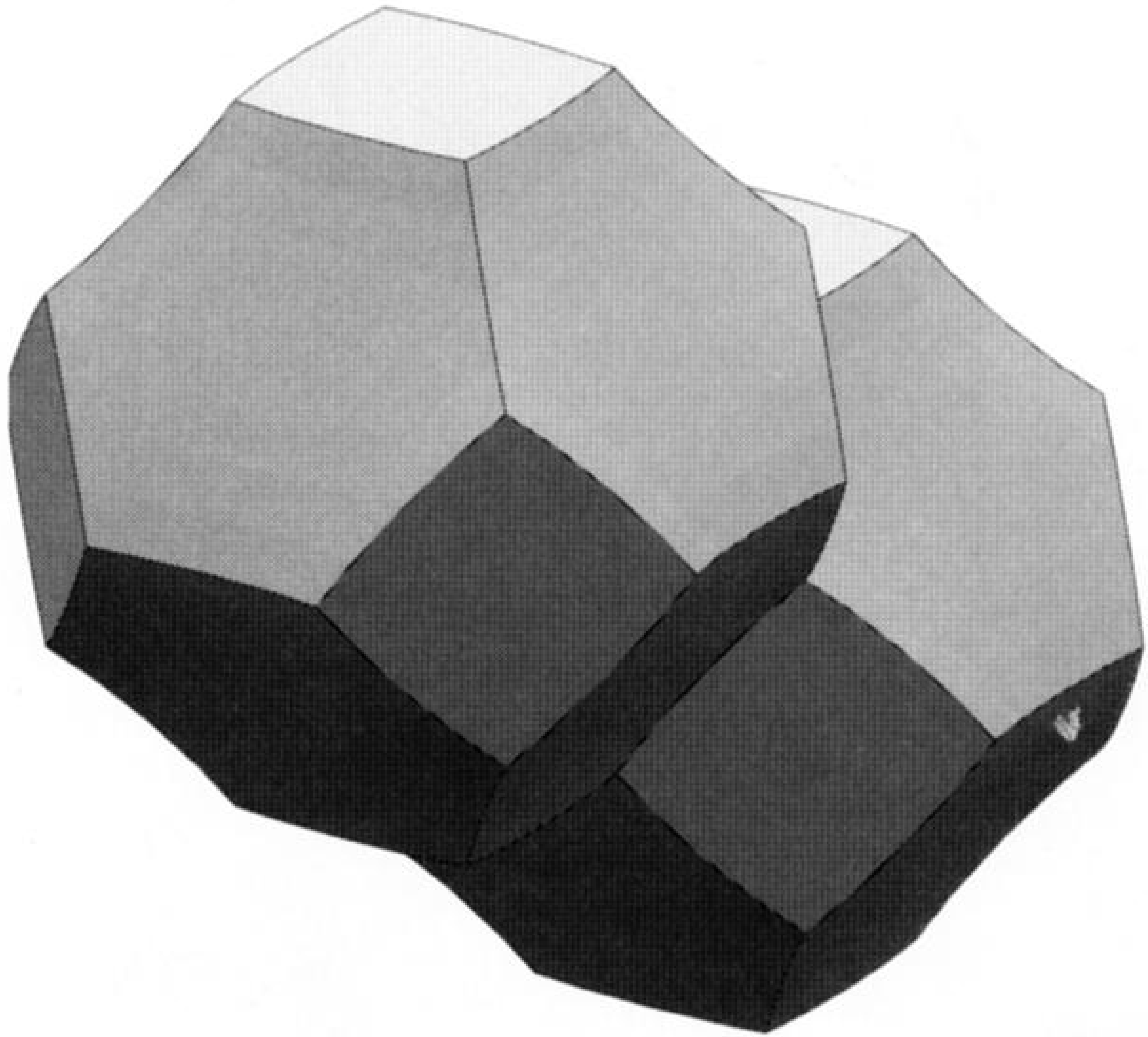

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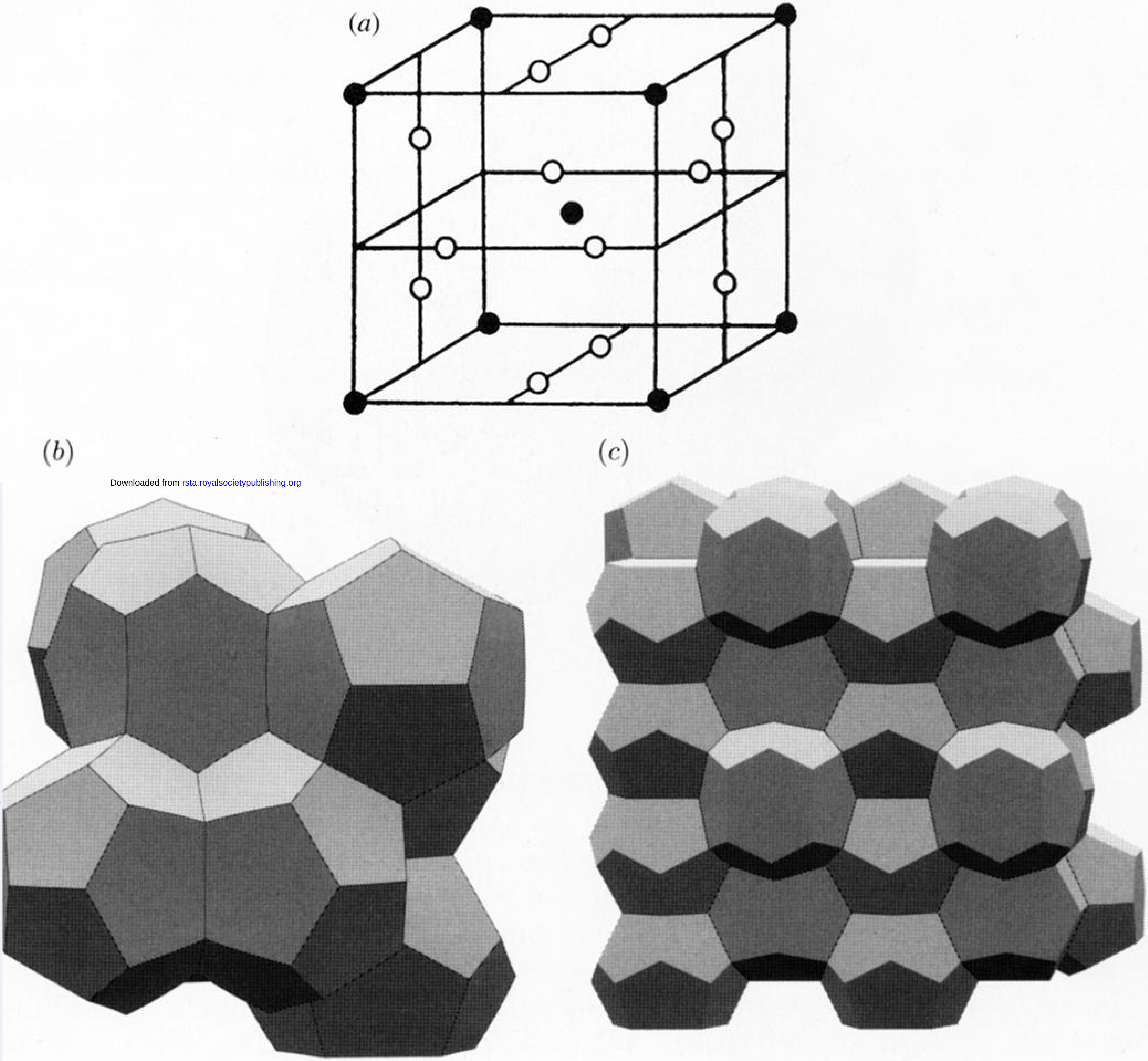

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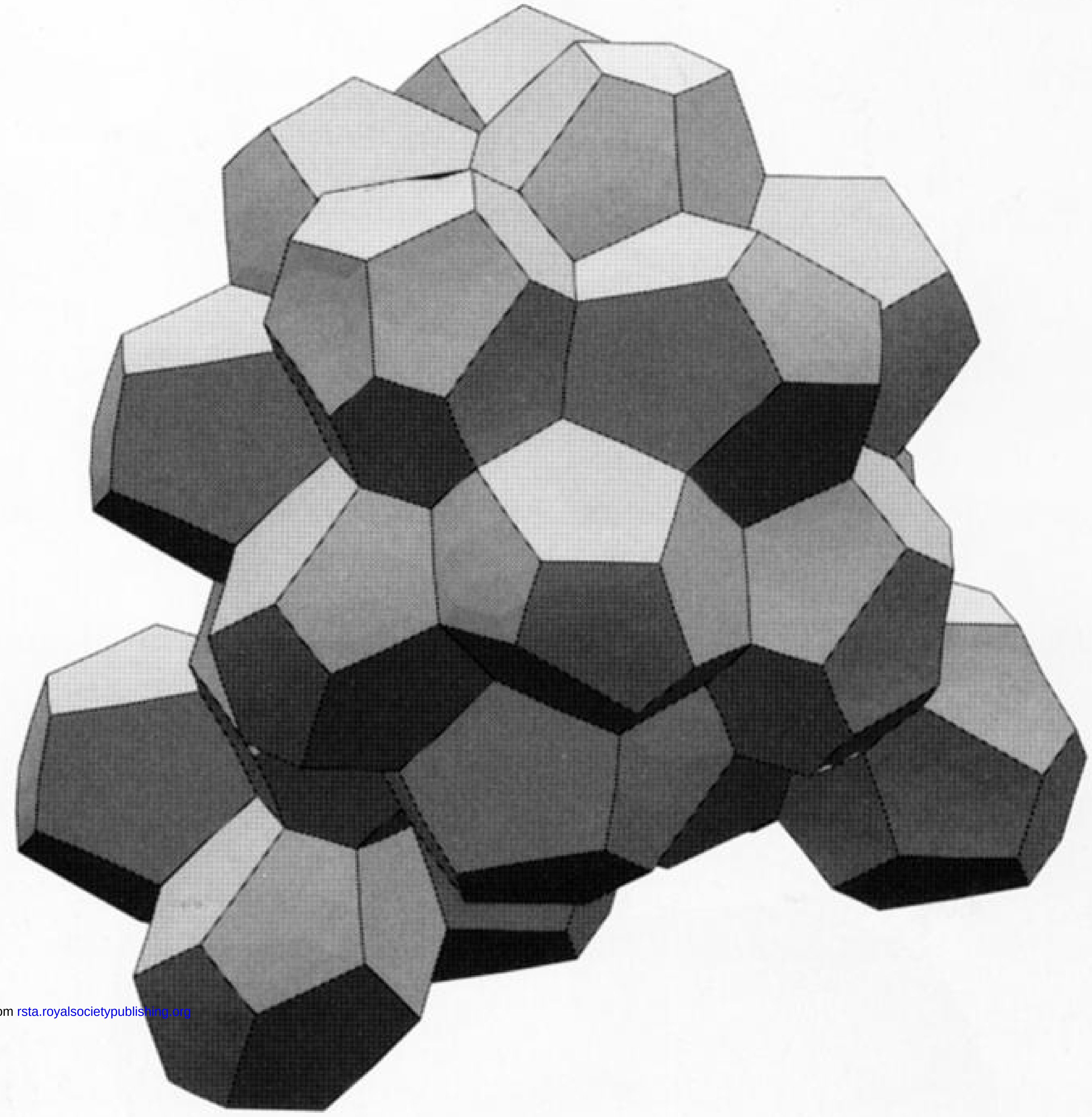

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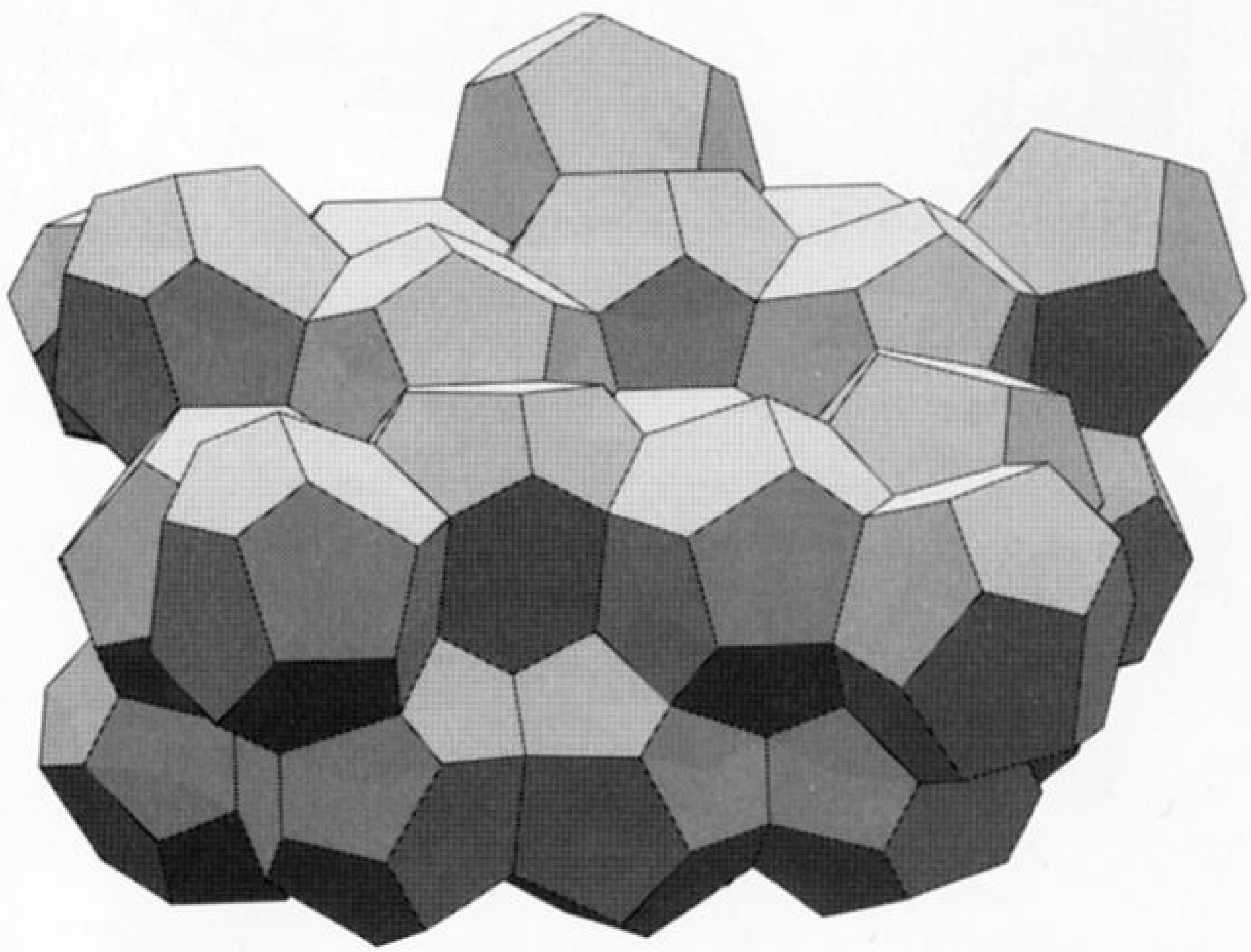

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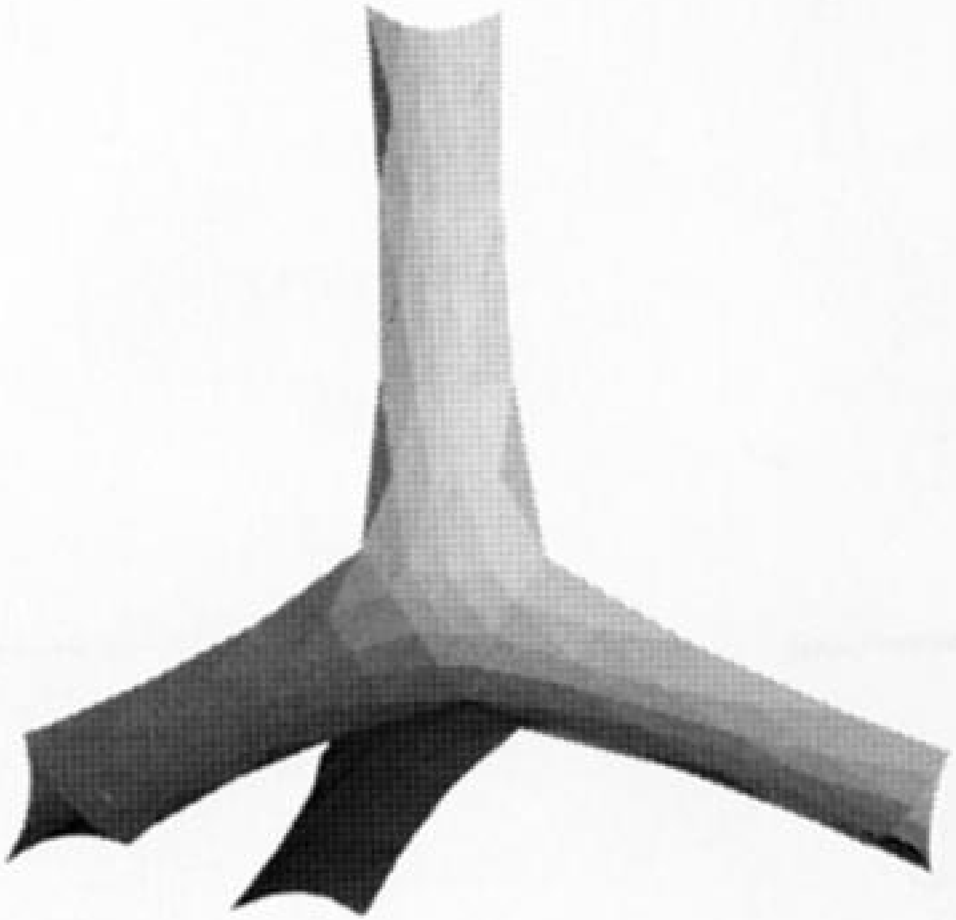

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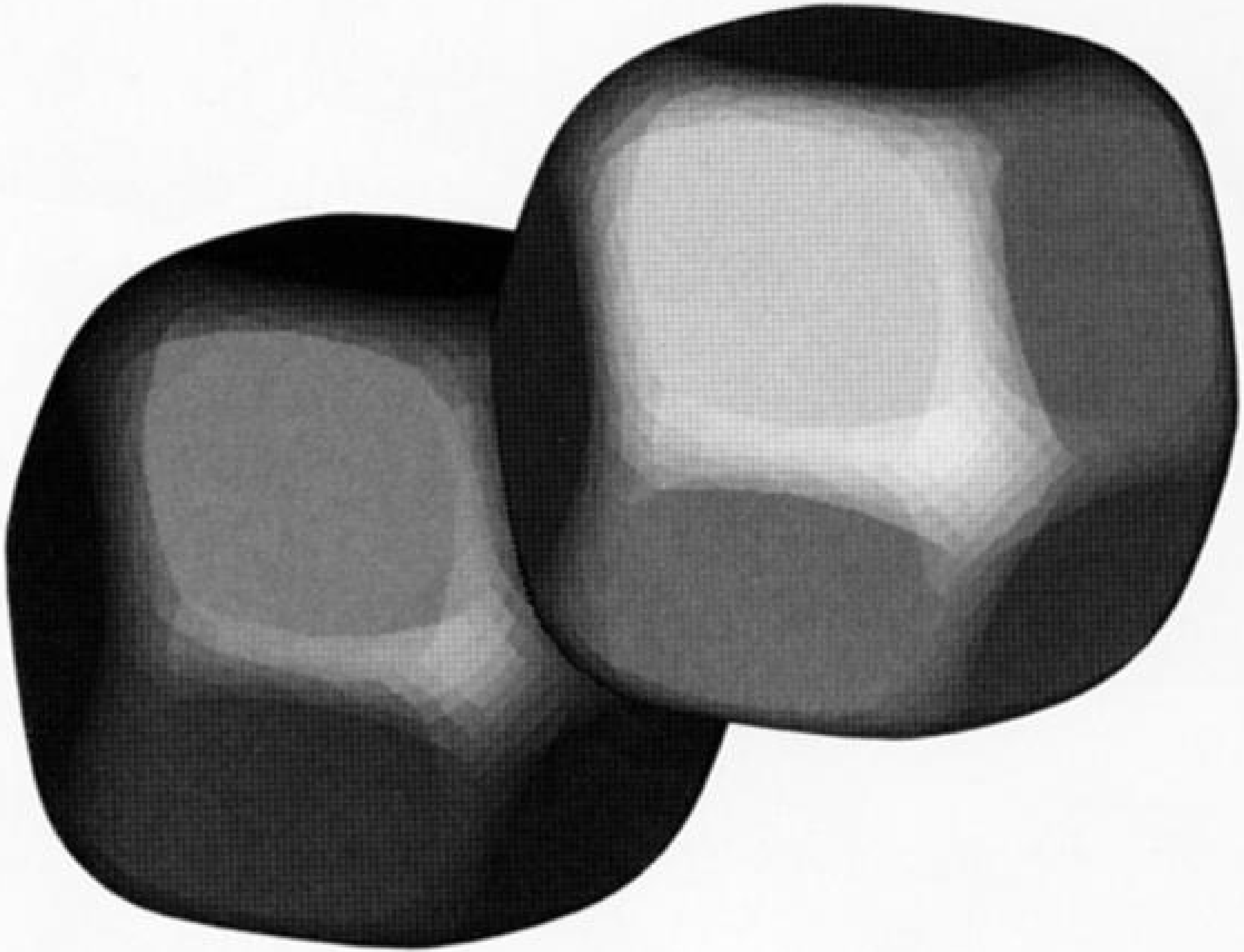

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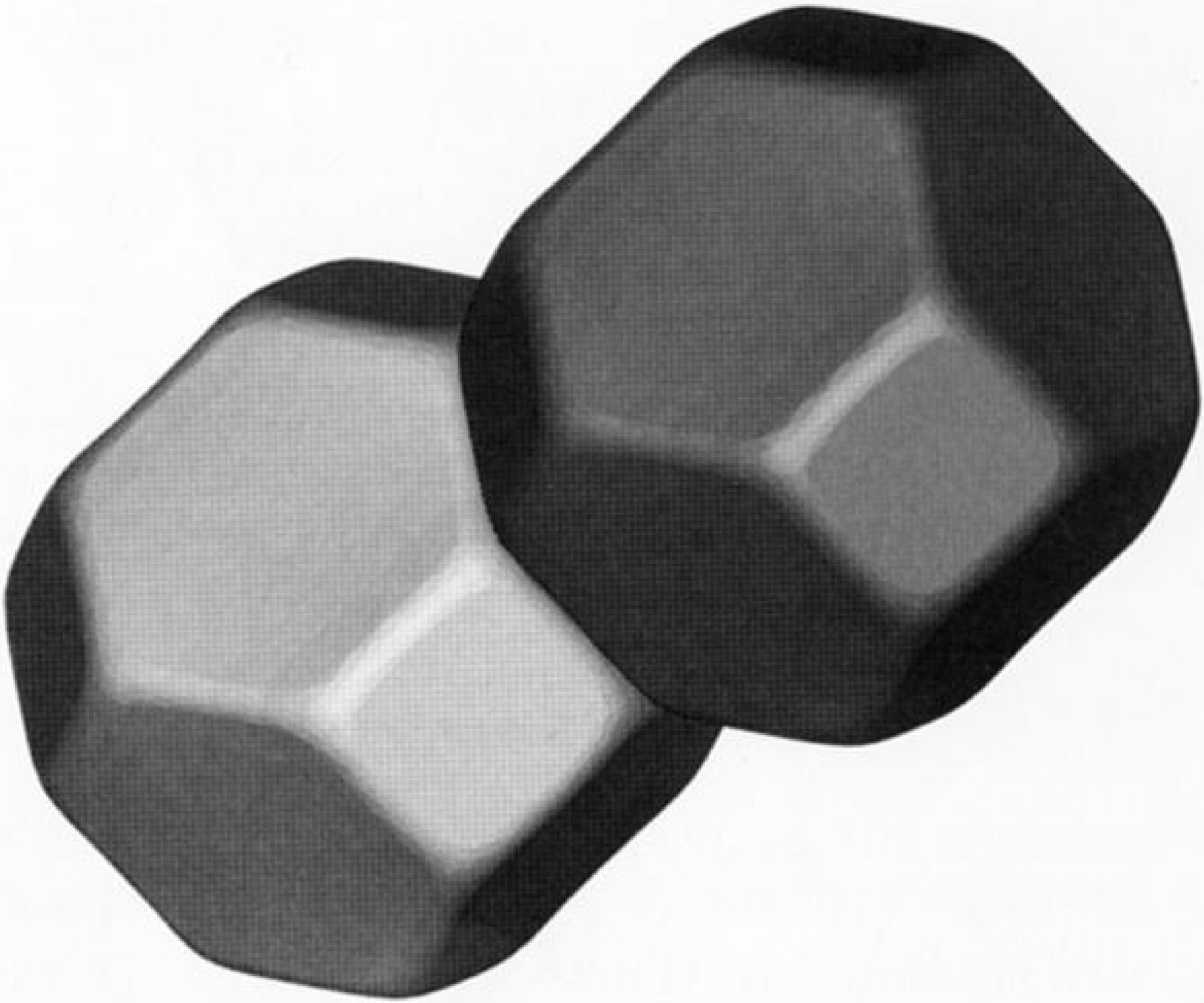

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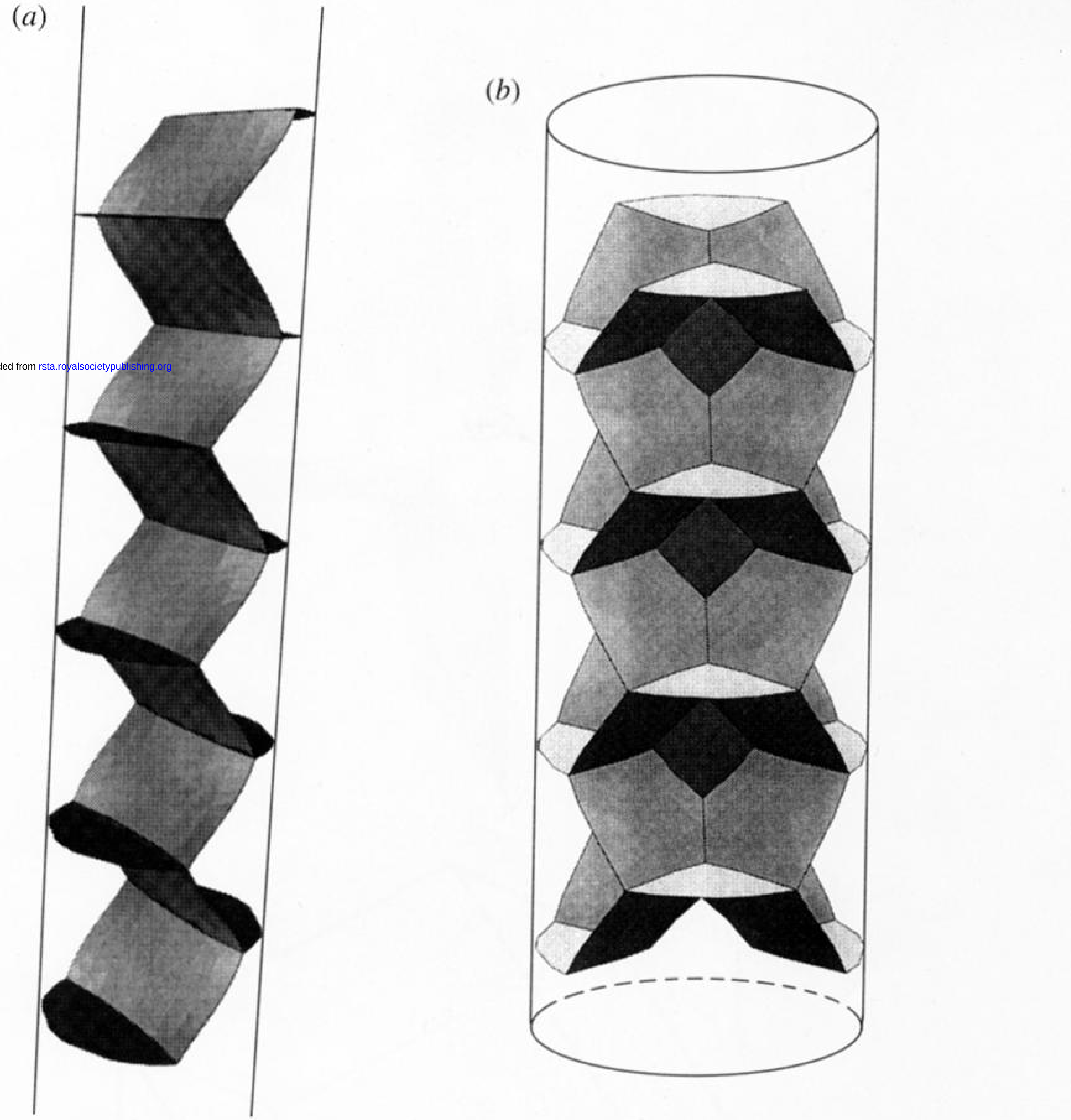

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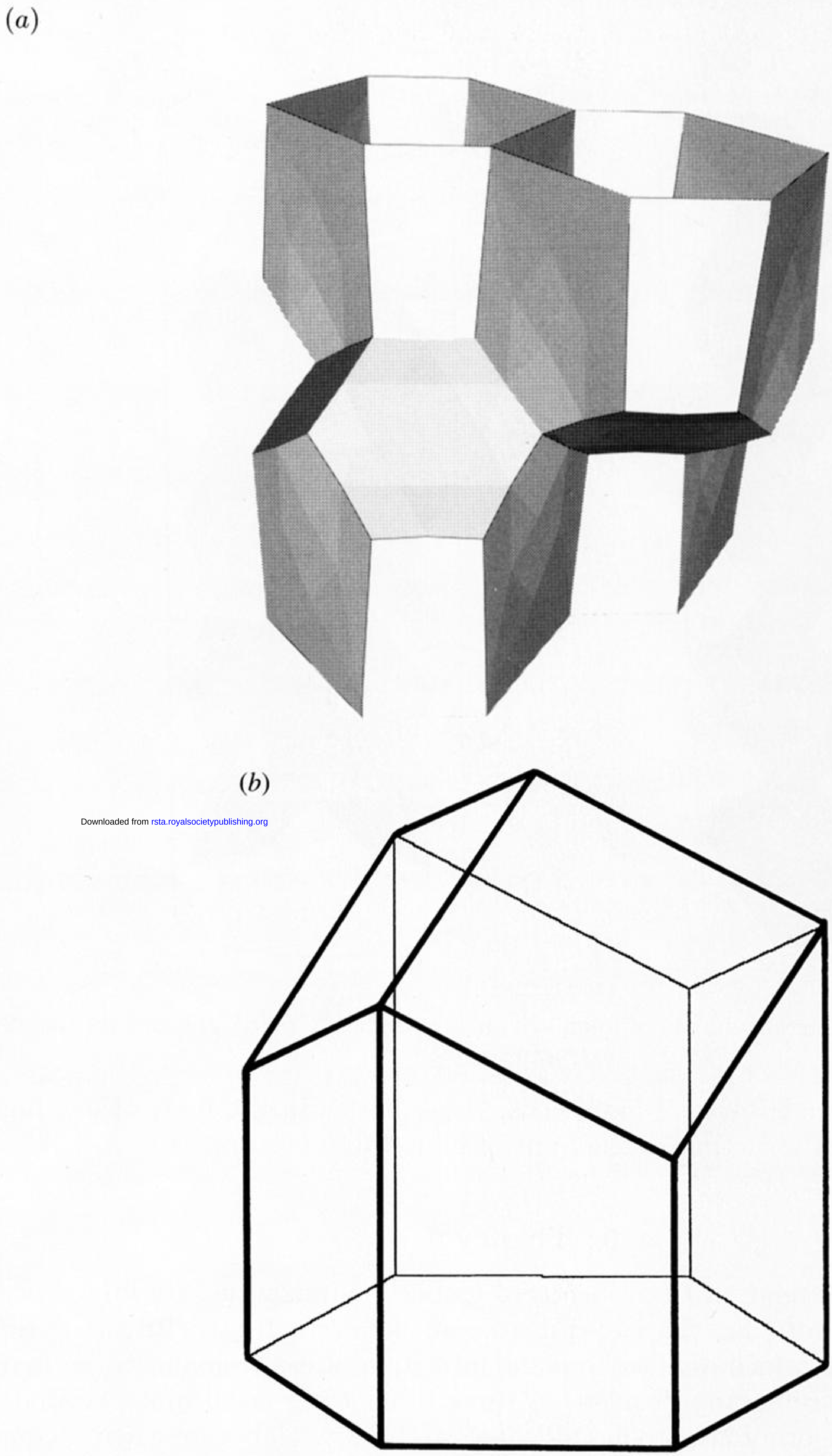

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