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Lithographite: A 5-,6-Connected Orthorhombic Structural Pattern in Space Group Pmmm

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Abstract-This paper describes the crystal structure of a novel, hypothetical 5-,6-connected orthorhombic structural pattern with the binary stoichiometry AB_2. The novel pattern lies in space group Pmmm, number 47. It possesses the Wells point symbol $(4^{10}6^2)(4^76^2)_2$ and has the Wellsean Schläfli index $(4^{2/5}, 5^{1/3})$. The pattern represents a fusing together of what are termed lithographene sheets. Such sheets can be envisioned as a projection of the lithographite lattice in (001), they represent a tiling of the Euclidean plane with hexagons and rhombi, where the rhombi have acute and obtuse angles of 60° and 120°, respectively, in the version of the structure reported in this paper. The lithographene sheet, which occurs in plane group p2mm, is compared to the ordinary graphene sheet in plane group p6mm.

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1. Introduction

In the course of investigating hypothetical structural modifications in the orthorhombic symmetry class, [1] one of the authors (MJB) discovered a novel 5-,6-connected structure-type with a binary stoichiometry AB_2. The new structure-type is named lithographite. An idealized illustration of the unit of pattern of this new structure-type, shown in plane projection in (001), is shown in Figure 1. Figure 2 shows an extended view of the lattice in plane projection in (001), such a pattern will be called a lithographene substructure of the layered lithographite lattice.

The lattice has been given the name lithographite because it is largely seen as a layering of a 2-dimensional lithographic tiling of the Euclidean plane by hexagons and rhombi. The dominant appearance of hexagons in this lithographene pattern is reminiscent of the much more symmetrical graphene sheet from which its name is also derived.

2. Lithographite

Referring to the unit cell of lithographite shown in plane projection in (001) in Figure 1, the white circles represent 6-connected distorted octahedral atoms, there is one such white circle, labeled A, per unit cell; while the black circles represent the 5-connected undistorted trigonal bipyramidal atoms, there are two such black circles, labeled B, per unit cell. This orthorhombic 5-,6-connected structural pattern, with binary stoichiometry AB_2, lies in space group Pmmm, number 47, with atoms in the following Wyckoff positions: the one 6-connected octahedral atom is in 1(a) (0, 0, 0), and the two 5-connected trigonal bipyramidal atoms are in 2(k) (x, 1/2, 0). For the special metric constraint in which the free parameter angle α, in Figure 1, is set exactly to 120°, the rhombi are of acute and obtuse angles of 60° and 120°, respectively [2].

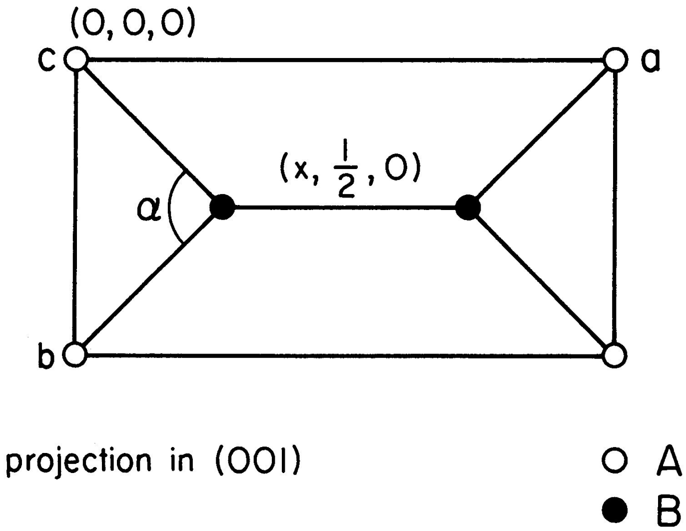

Figure 1: View of unit cell of lithographite in (001).

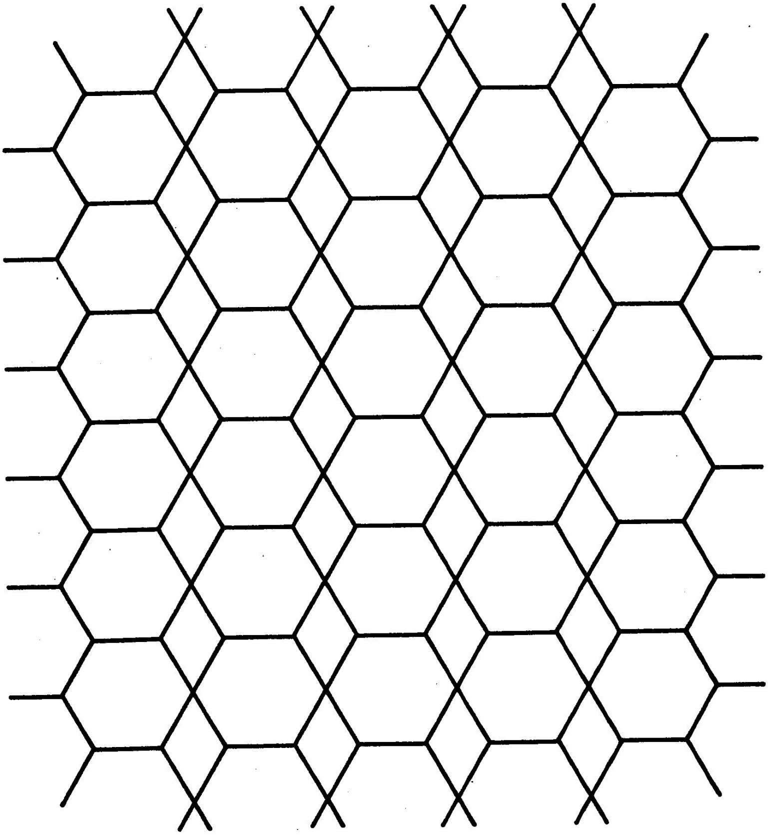

Figure 2: Extended view of lithographite in (001) projection, the crystalline litographite lattice possesses the Wells point symbol $(4^{10}6^{2})(4^{7}6^{2})_{2}$ and belongs to the symmetry space group Pmmm, while the Wells point symbol for the sheet (shown here) is given by $(4^{2}6^{2})(4.6^{2})_{2}$ and it belongs to the plane group p2mm.

Topologically, the crystalline lithographite lattice possesses the Wells point symbol $(4^{10}6^2)(4^76^2)_2$ and has the Wellsean Schläfli index $(4^{2/5}, 5^{1/3})$. For further explanation of the enumeration of the Wells point symbols for crystalline structures, and their subsequent translation into the corresponding Schläfli indices, and the importance of the Schläfli indices in uncovering fundamental topological and geometrical information about crystalline structures, the reader is referred to the earlier installments in this series by the authors [3]. It is interesting in this regard that such an apparently simple filling of space by the alignment of these familiar lithographene sheets in 3D can lead to such a complex compound topology as that indicated by the Wells point symbol for the network above.

3. Lithographene Sheets

Referring to the extended drawing of lithographite shown in plane projection in (001) in Figure 2, one can see that this sheet by itself represents a familiar, classical and decorative tiling of the Euclidean plane with hexagons in strips that are so aligned with parallel hexagons in strips that rhombi are inscribed in the areas where the fused hexagons have frustrations. If we set the free parameter α equal to 120°, the internal hexagonal angles are ideal at 120° and the lattice parameters are constrained to a fixed ratio of **a/b** = $2/3^{1/2}$.

By removing all of the neighboring lithographene layers in lithographite away from each other, one has transformed the octahedral vertices in lithographite into distorted square planar 4-connected vertices in the lithographene sheet, by truncation. Similarly, the trigonal bipyramidal vertices of lithographite have been transformed into ideal trigonal planar 3-connected vertices in the lithographene sheet. This lithographene pattern is thus a 3-,4-connected plane net. The Wells point symbol for the sheet is given by $(4^26^2)(4.6^2)_2$. One can see immediately that this is the point symbol, like the corresponding one for the 3D lithographite lattice above, for a so-called Wellsean network [3]. Alternatively, lithographene (or lithographite) can be described as having the Wells point symbol for a topologically irregular pattern, and its respective Schläfli index is thus given by $(5^{1/5}, 3^{1/3})$. In comparison to this topology, one can consider the graphene sheet with its regular (Platonic) topology of 6^3 or (6, 3).

The construction of the lithographene sheet from the graphene sheet can easily be envisioned, the latter sheet is shown in Figure 3.

In both structures, one has strips of hexagons that are fused into each other. The difference is in the alignment of the hexagon strips, for in the grapheme sheet the strips are completely regularly connected into each other leading to a high topology, a high plane group symmetry of p6mm and the absence of any frustrations [4]. This is achieved by aligning the hexagon strips such that hexagons from one strip are related to hexagons from the next-to-nearest strips by a reflection mirror plane, m. Therefore we have in the graphene sheet, every other strip of parallel hexagons related by a mirror plane through the intervening strip of hexagons to every other strip of parallel hexagons. In contrast, in the lithographene sheet the topology is Wellsean or irregular, the symmetry of its plane group is lowered to p2mm, and the alignment of its hexagon strips leads to the introduction of rhomboid frustrations. The great contrast can be understood in terms of the alignment of the strips of hexagons in the latter situation, for in lithographene each and every parallel hexagon strip is related to every other one, including its adjacent neighbors, by reflection symmetry planes, m, passing between and also through the hexagon strips [4].

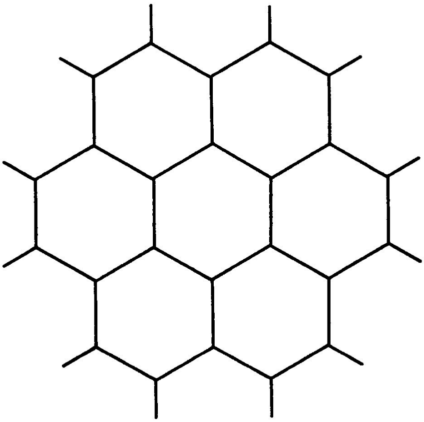

Figure 3: View of the much more symmetrical and regular graphene sheet with corresponding Wells point symbol 6^3 that belongs to the corresponding symmetry plane group p6mm.

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