[CONTRIBUTION FROM THE CHEMICAL LABORATORY OF THE UNIVERSITY OF CALIFORNIA]

ELECTRONIC STRUCTURES OF CRYSTALS. I[1]

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In another article[3] the author has extended the Lewis theory of atomic structure[4] to include all the elements, the structures obtained being based largely on the ideas (1) that the electrons around an atomic nucleus (except the two in the innermost shell) are in groups of 2 and, in the inner shells of the heavier elements, 3 electrons, (2) that these groups are at the corners of more or less regular polyhedra around the nucleus, and (3) that each group (excepting those in the innermost polyhedron) occupies a position opposite a face of the next inner shell.

As a corollary of this theory, when 2 atoms are joined by a single bond, the bond electron pair should tend to place itself on (or near, if one or the other of the kernels is unsymmetrical) the straight line joining the atomic centers and opposite a face of the outermost kernel polyhedron[5] of each atom joined by the bond. In this paper it will be shown that in a large number of crystals the atoms are joined by single bonds of this type, the number and arrangement of these bonds being in full accord with the atomic structures proposed.

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[1] This paper (except for unimportant changes) was written in 1920, but unavoidable circumstances have delayed its publication.

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[3] Huggins, *Science*, **55**, 459 (1922); *J. Phys. Chem.*, October, 1922.

[4] Lewis, THIS JOURNAL, **38**, 762 (1916).

[5] This rule does not, of course, determine the arrangement of valence electrons around a kernel of an element in the first row of the periodic table.

Diamond.[6]—The structure of the diamond crystal is shown in Fig. 1. Each atom is symmetrically surrounded by 4 others, at tetrahedron corners.
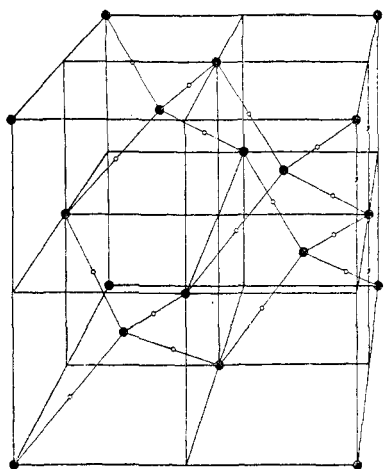

Fig. 1.—Arrangement of atomic centers and valence electron pairs in a unit cube of the diamond crystal.

Since each carbon has 4 valence electrons which (from atomic theory and from the facts of organic chemistry) tend to be arranged in tetrahedral fashion around the kernel, pairing whenever possible with single electrons from other atoms (to form a "group of 8" or "octet" around each atom), we can feel certain that these valence electrons are *in pairs on the center lines*[7] between adjacent atoms, and since all the atoms are identical, each "bond electron pair" must be midway between the centers of the 2 atoms it joins. Each atom is held in place by 4 carbon-carbon single bonds of the ordinary type familiar to organic chemists. The well-known difficulty of breaking such bonds is undoubtedly the cause of the extreme hardness of this substance.

Silicon,[8] Germanium,[9] Tin.[10]—Silicon, germanium and gray tin form crystals in which the atoms are marshaled exactly as in diamond. The electronic structures of atoms of these elements, according to the author's theory, may be represented as follows: Si, $(+ 14) (2 \times 1) (4 \times 2) (4)$; Ge, $(+ 32) (2 \times 1) (6 \times 3) (4 \times 2) (4)$; Sn, $(+ 50) (2 \times 1) (8 \times 3) (6 \times 2) (4 \times 2) (4)$. In each of these formulas the first parenthesis encloses the nuclear charge, the last the number of valence electrons, and those between indicate the number of groups and the number of electrons in each group in

[6] (a) W. H. and W. L. Bragg, *Proc. Roy. Soc.*, **89A**, 277 (1913); (b) "X-Rays and Crystal Structure," G. Bell and Sons, London, 1916, p. 102. (c) W. H. Bragg, *Proc. Phys. Soc. (London)*, **33**, 304 (1921). (d) Hull, *Phys. Rev.*, [2] **10**, 695 (1917). (e) Huggins, *ibid.*, [2] **18**, 333 (1921); (f) [2] **19**, 346 (1922).

[7] If the valence shells were *cubes of single electrons*, adjacent atoms having cube edges in common, it can be shown that the resulting structure should have tetragonal symmetry. Since this is not the case, if each atom has a shell of 8 electrons, they *must* be *in pairs at tetrahedron corners on the lines joining atomic centers*. Similar reasoning with regard to the other crystals to be considered shows that in each case the *pair* of valence electrons is the unit.

[8] (a) Debye and Scherrer, *Physik. Z.*, **17**, 277 (1916). (b) Hull, *Phys. Rev.*, [2] **9**, 566 (1917). (c) W. H. Bragg, *Proc. Phys. Soc. (London)*, **33**, 222 (1921). (d) Gerlach, *Physik. Z.*, **22**, 557 (1921); (e) Gerlach, *ibid.*, **23**, 114 (1922).

[9] Hull, Am. Phys. Soc. Meeting, Washington, D. C., April, 22, 1922.

[10] Bijl and Kolkmeijer, *Chem. Weekblad*, **15**, 1077, 1264 (1918); *Proc. Acad. Sci. Amsterdam*, **21**, 494, 501 (1919).

each kernel shell, in order from the nucleus out.   Thus in a tin atom we have: nucleus; first shell, two single electrons; second shell, a cube of triplets; third shell, an octahedron of pairs (one pair opposite each of the cube faces); fourth shell, a tetrahedron of pairs (opposite half of the 8 octahedron faces); fifth shell, 4 valence electrons.

The valence electrons in each atom, according to the present theory, pair off with valence electrons in the surrounding atoms, the pairs thus formed arranging themselves tetrahedrally opposite the faces of the outer kernel tetrahedra.[7]   These crystals then possess the same arrangement of valence electrons, as well as of atomic nuclei, as diamond.

Since the marshaling of the other electrons in each atom relative to the valence electrons is known (assuming the atomic structures assigned them to be correct), it is possible to obtain the approximate position of every electron in the crystal.   This is also the case for the other crystals to be considered.

Zinc Sulfide,[11] Cuprous Chloride,[12] Cuprous Bromide,[12] Cuprous Iodide,[12] Silver Iodide.[13]—The cubic crystals of zinc sulfide (sphalerite), cuprous chloride, bromide and iodide, and silver iodide possess structures like that of diamond (considering atomic centers only) except that half of the carbon atoms are replaced by metal atoms and half by sulfur or halogen atoms, in such a way that each electropositive atom is symmetrically surrounded by 4 electronegative atoms, at tetrahedron corners, and *vice versa*.

The atomic formulas of the elements in these crystals are: Zn, $(+ 30)$ (2×1) (6×3) (4×2) (2); Cu, $(+ 29)$ (2×1) (6×3) (4×2) (1) Ag, $(+ 47)$ (2×1) (8×3) (6×2) (4×2) (1); S, $(+ 16)$ (2×1) (4×2) (6); Cl, $(+ 17)$ (2×1) (4×2) (7); Br, $(+ 35)$ (2×1) (6×3) (4×2) (7); I, $(+ 53)$ (2×1) (8×3) (6×2) (4×2) (7).   The outermost kernel shell is in each case a tetrahedron.   In each of the compounds under discussion there are 8 valence electrons "per molecule," an average of 4 per atom, precisely the number required for a pair on each center line[14] between adjacent atoms.   Such an arrangement gives a complete valence tetrahedron around each atom and places each pair opposite a face of the outer kernel shell in each of the two atoms it bonds together.

It may be noted that in order to obtain these structures either from the simple molecules, Zn :S:, Cu :Cl:, etc., or from the ions, Zn^{++}, :S:$^{--}$, Cu^+, :Cl:$^-$, etc., a bond must be formed by the addition of an atom

[11] (a) W. H. Bragg and W. L. Bragg, *Proc. Roy. Soc.*, **88A**, 428 (1913); **89A**, (b) 248, (c) 277, (d) 468 (1913); (e) Ref. 6 b, p. 97.   (f) Ewald, *Ann. Physik*, [4] **44**, 257 (1914).(g) Ref. 6 e.

[12] Wyckoff and Posnjak, THIS JOURNAL, **44**, 30 (1922).

[13] Wilsey, *Phil. Mag.*, [6] **42**, 262 (1921).

[14] These pairs would not be at the *mid-points* of the center lines, of course.   The reasoning in Ref. 7 in regard to the pairing of valence electrons applies here, also.

containing a "lone pair" (one not acting as a bond) to one which is capable of adding that lone pair to its valence shell. Reactions of this type are of great importance in crystal formation. In fact the formation of inorganic crystals other than the metals, the alkali halides, and the alkaline earths, consists chiefly of reactions of this type, as indicated by the structures of the substances before and after crystallization.

Zinc Sulfide,[15] Zinc Oxide,[16] Cadmium Sulfide,[15] Silver Iodide.[17]—The hexagonal crystals of zinc sulfide (wurzite), zinc oxide, cadmium sulfide and silver iodide have atomic arrangements very similar to that of the foregoing crystals. Each metal atom is surrounded by 4 practically equidistant[18] tetrahedrally disposed oxygen, sulfur or iodine atoms, and vice versa.

The atomic formulas of oxygen and cadmium are: O, $(+ 8)$ (2×1) (6); Cd, $(+ 48)$ (2×1) (8×3) (6×2) (4×2) (2). Each oxygen atom, according to the Lewis theory, tends to add 2 valence electrons to complete a tetrahedron of pairs around the kernel. The author's theory indicates that the cadmium kernel also tends to surround itself with a tetrahedron of electron pairs, with one pair opposite each face of the kernel tetrahedron.

There are just enough valence electrons in each of these crystals also, for a pair on each center line between adjacent atoms, and in such a disposition there is a tetrahedron of pairs around each kernel, as required by the theory.[19]

Silicon Carbide, SiC.[20]—Crystals of silicon carbide (carborundum) may, according to Hull, be composed of structures of either of the preceding two types. Since there are 4 valence electrons per atom and since the tetrahedron of pairs is the stable form for the valence shell of an atom of either element, we are again justified in assuming that the valence electrons are in pairs on the lines connecting neighboring atomic centers.

Chalcopyrite, $CuFeS_2$.[21]—In chalcopyrite the atomic centers are distributed very nearly as in the diamond structure, the atoms of carbon

[15] Ref. 6b, p. 227. W. L. Bragg, Phil. Mag., [6] 39, 647 (1920).

[16] Ref. 15. Also Aminoff, Z. Krist. Mineralog., 56, 495 (1921); 57, 204 (1922).

[17] Aminoff, Z. Krist., 57, 180 (1922).

[18] Since the structure does not possess tetrahedral symmetry around any atom, one of the 4 surrounding atoms is slightly closer to or further away from a given atomic center than the other 3.

[19] It would be absolutely impossible for each sulfur, oxygen or iodine kernel in these crystals to be surrounded by a cube of single electrons and be bonded through the cube edges to the surrounding metal atoms. Hence this is clearly a case where the "cubical atom" will not fit the observed facts. See Ref. 7.

[20] Burdick and Owen, THIS JOURNAL, 40, 1749 (1918). Hull, Phys. Rev., [2] 13, 292 (1919); 15, 545 (1920). Espig, Abhandl. Math.-Phys. Klasse Sächs. Akad. Wiss. Leipzig, 38, 53 (1921).

[21] Burdick and Ellis, THIS JOURNAL, 39, 2518 (1917).

being replaced by those of other elements in such a way that each metal atom is surrounded by 4 equidistant sulfur atoms at corners of a nearly regular tetrahedron, and each sulfur atom by 4 metal atoms (2 Cu and 2 Fe) also tetrahedrally arranged.[22]

The most probable formulas for the copper and iron atoms in this crystal are the following: Cu, (+ 29) (2 × 1) (5 × 3 + 1 × 2) (4 × 2) (2);[23] Fe, (+ 26) (2 × 1) (2 × 3 + 4 × 2) (4 × 2) (2).[23]   There are in this case 16 valence electrons per molecule, which is again 4 per atom, just the number required to place them in pairs on the center lines, opposite the faces of the kernel tetrahedra, as in the previously considered crystals.

Iron **Disulfide**.—In pyrite,[24] the cubic form of iron disulfide, each iron atom is surrrounded by 6 sulfur atoms at the corners of a nearly regular octahedron and each sulfur by 4 tetrahedrally disposed atoms, 3 being iron and 1 sulfur.   Each sulfur atom we can reasonably assume to have 6 valence electrons of its own and to add 2 from another atom or atoms so as to complete a tetrahedron of pairs around it,—one pair on or near the straight lines between each sulfur nucleus and the 4 surrounding atoms.   In order that this may be the case each iron atom must furnish 2 valence electrons.[25]
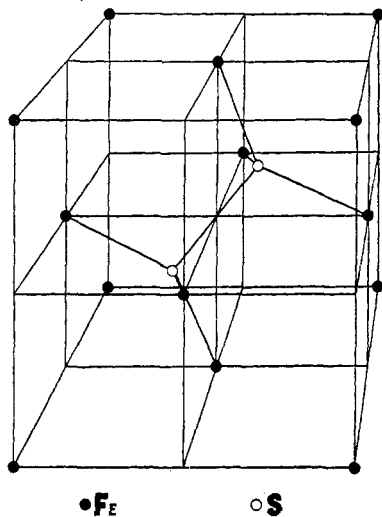
Fig. 2.—Arrangement of iron atoms around each S-S group in a crystal of pyrite (FeS₂).

●F$_E$ ○S

In this assemblage each iron kernel is surrounded by an octahedron of electron pairs, an indication that the atomic structure is probably that represented by the formula, (+ 26) (2 × 1) (6 × 3 + 2 × 2) (2), in which

[22] Burdick and Ellis place the (001) sulfur planes exactly midway between the copper and iron planes, making the distance between centers of sulfur and copper atoms precisely the same as that between sulfur and iron centers.   This can be the case only if the iron and copper atoms have exactly the same attraction for electrons (or, in other words, if their "atomic radii" are the same), which is highly improbable.   We may be quite certain, therefore, that the sulfur plane is slightly closer to either the iron or the copper plane.   That this is correct is shown by the failure of these investigators to obtain reflections corresponding to ¹/₂ the distance between sulfur planes.

[23] (a × 3 + b × 2) here means a kernel shell consisting of a electron triplets and b electron pairs, these 6 groups being at corners of a more or less distorted octahedron.

[24] (a) Ref. 11d.   (b) Ref. 6b, p. 127.   (c) Ewald, *Physik. Z.*, **15**, 399 (1914).   (d) Ewald and Friedrich, *Ann. Physik*, [4] **44**, 1183 (1914).   (e) Ref. 6e.

[25] This confirms the divalence of iron in this substance, which is indicated by the fact that oxidation gives *ferrous* sulfate.

the outer kernel shell is a distorted cube, (instead of a tetrahedron, as in CuFeS$_2$).[26]

In marcasite,[27] the rhombic form of iron disulfide, there is a similar arrangement of atoms (and so of electrons) around each atom, although the distortions from the regular octahedral and tetrahedral arrangement are somewhat greater.

Disulfides and Diarsenides.—Other substances which are crystallographically very similar[28] to pyrite, and which in all probability possess the same marshaling of atomic centers, are hauerite, MnS$_2$;[29] nickeliferous var, (Fe,Ni)S$_2$; arsenoferrite, FeAs$_2$; smaltite, CoAs$_2$; and cloanthite, NiAs$_2$.[30] Like marcasite[28] are loellingite, FeAs$_2$;[27] safflorite, CoAs$_2$; and rammelsbergite, NiAs$_2$.

In each of the foregoing sulfides, in order to give the same electronic structure as in pyrite or marcasite, the metal atoms must supply *two* valence electrons each. In the diarsenides, since each arsenic atom can furnish only 5 valence electrons, *four* must come from each metal atom. The probable atomic formulas are: Mn, (+ 25) (2 × 1) (5 × 3 + 3 × 2) (2); Fe, (+ 26) (2 × 1) (6 × 3 + 2 × 2) (2), and (+ 26) (2 × 1) (4 × 3 + 4 × 2) (4); Co, (+ 27) (2 × 1) (5 × 3 + 3 × 2) (4); Ni, (+ 28) (2 × 1) (8 × 3) (2), and (+ 28) (2 × 1) (6 × 3 + 2 × 2) (4); As, (+ 33) (2 × 1) (6 × 3) (4 × 2) (5).

Cobaltite and Similar Compounds.—Cobaltite, CoAsS, has been shown by the Braggs[31] to have a structure like that of pyrite, the iron being replaced by cobalt and half of the sulfur by arsenic atoms. Other substances which are crystallographically very similar and which, doubtless, have the same marshaling of atoms and valence electrons are willyamite, CoSbS; gersdorffite, NiAsS; ullmanite, NiSbS; and kallilite, NiBiS. Closely resembling marcasite are the minerals arsenopyrite, FeAsS;[27] glaucodotite, xCoAsS.yFeAsS; and wolfachite, NiAsS. Each arsenic, antimony or bismuth atom in these crystals furnishing 5 valence electrons and each sulfur 6, each metal atom must supply 3, there being then an electron pair on (or near) each center line.

The formulas representing the probable structures of the elements in

[26] In some substances an electropositive atom having a tetrahedron as its outermost kernel shell may be surrounded by a valence octahedron (in which case *kernel* pairs are opposite half of the faces of the valence shell), if the valence pairs are pulled sufficiently far away from the kernel by electronegative atoms. If this were the case in pyrite, however, we should expect similar disulfides of metals like copper and zinc, in which the outermost kernel shell is always a tetrahedron.

[27] Huggins, *Phys. Rev.*, [2] **19**, 369 (1922).

[28] Groth, "Chemische Krystallographie," Wm. Engelmann, Leipzig, 1906, vol. I. Wherry, *J. Wash. Acad. Sci.*, **10**, 487 (1920).

[29] Ref. 6b, p. 154.   Ref. 24c and d.

[30] Perhaps also laurite, RuS$_2$; and sperrylite, PtAs$_2$.

[31] Ref. 6 b, p. 154.

these compounds (except those of sulfur and arsenic, which have been given) are: Fe, (+ 26) (2 × 1) (5 × 3 + 3 × 2) (3); Co, (+ 27) (2 × 1) (6 × 3 + 2 × 2) (3); Ni, (+ 28) (2 × 1) (7 × 3 + 1 × 2) (3); Sb, (+ 51) (2 × 1) (8 × 3) (6 × 2) (4 × 2) (5); Bi, (+ 83) (2 × 1) (8 × 3) (6 × 3) (8 × 2) (6 × 3) (5).

Arsenic, Antimony, Bismuth.—An atom of arsenic, antimony or bismuth has 5 valence electrons. These tend to complete a tetrahedron of pairs by adding 3 electrons from other atoms. Three of the 4 valence pairs around a given atom are, therefore, *bond* pairs and one a *lone* pair. The disposition of atomic centers in crystals of the elements[32] fully bears out this view. As shown in Fig. 3a, which has been taken in part from an article by James and Tunstall,[32] each atom (such as F) is surrounded by 3 equi-

• Nucleus.
· Electron pair.
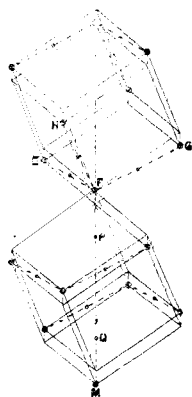
●Atomic nucleus.   ○Electron pair.

Fig. 3a.—Arrangement of atomic centers and valence electron pairs in a crystal of As, Sb or Bi.
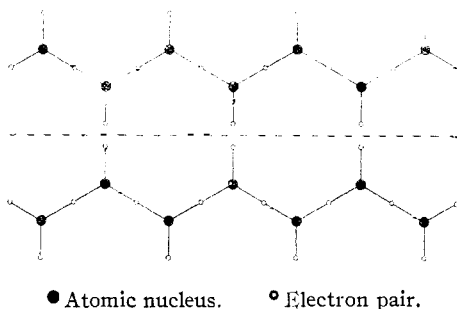
Fig. 3b.—A 2-dimensional representation of the arrangement in a crystal of As, Sb or Bi.

distant atoms, at corners of a distorted tetrahedron. Five electrons for each atom can be arranged in this structure, in accord with its symmetry, in but one way, so that there is one (bond) pair on each center line (FE, FG, FH, etc.) between *nearest* atoms and 2 (lone) pairs (P, Q) between adjacent atoms on each of the long diagonals (FM) of the unit rhomb.

It should be noted that the mutual repulsion between atoms E, G and H, unbalanced by the repulsion from a fourth atom equidistant from F, forces them away from the arrangement at 3 corners of a *regular* tetrahedron with F at the center.

[32] The structure of antimony has been determined by James and Tunstall, *Phil. Mag.*, [6] **40**, 233 (1920) and by Ogg, *ibid.*, [6] **42**, 163 (1921). See also Ref. 6 b, p. 227. The bismuth structure has been reported by Ogg, *loc. cit.*, by James, *Phil. Mag.*, [6] **42**, 193 (1921), and by Kahler, *Phys. Rev.*, [2] **18**, 210 (1921). Arsenic is so similar crystallographically that there can be no doubt but that it possesses the same type of structure.

The important features of the structure may be readily visualized by a consideration of Fig. 3b, which represents an imaginary similarly constituted *two*-dimensional crystal. The dotted line shows how cleavage occurs, between the lone pairs (P, Q, etc.), in such a way as not to break any single bonds (of the FE, FG, FH type).

Quartz.—The disposition of atoms and electrons in quartz has been reported by the author in another paper.[33] Each silicon kernel is surrounded by 4 valence pairs at tetrahedron corners, bonding it to 4 oxygen kernels; and each oxygen kernel is surrounded by 4 tetrahedrally-arranged pairs, 2 of these serving as bonds to the 2 adjacent silicon atoms and 2 being lone pairs.

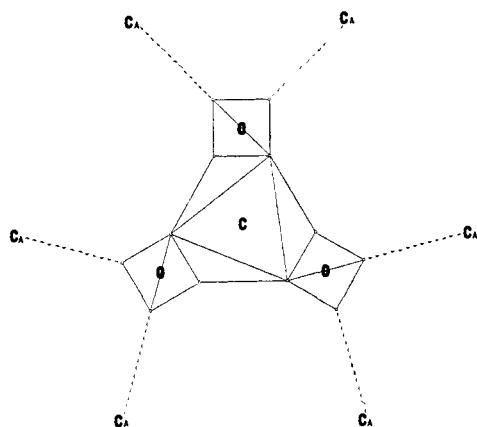Calcium Carbonate.—In a calcite crystal[34] each calcium atom is at the center of an octahedron of 6 equivalent oxygen atoms; each carbon is surrounded by 3 equidistant oxygen atoms at the corners of an equilateral triangle, and each oxygen by two equidistant calciums and one carbon.

From the atomic structures, Ca, (+ 20) (2 × 1) (8 × 2) (2), C, (+ 6) (2 × 1) (4); O, (+ 8) (2 × 1) (6); we see that there is a total of 24 valence electrons for each $CaCO_3$ "molecule." The only way in which these can be logically arranged in accord with the symmetry around each atom[35] is that represented in Fig. 4. There is an octahedron of pairs around each calcium atom, connecting it by single bonds to the surrounding oxygens. An octahedron of pairs is also around each carbon, bonding it by *double* bonds to the 3 oxygens around it. Each oxygen is surrounded by a tetrahedron of pairs, bonding it to two calciums and (by a double bond) to one carbon.

Fig. 4.—Arrangement around each carbon atom in calcite.

A similar arrangement of atoms and of electrons exists in aragonite,[36] the rhombic form of $CaCO_3$, although the valence tetrahedra and octahedra are more distorted.

Similar Carbonates and Nitrates.—The atoms and valence electrons in

[33] Ref. 6f, p, 363.

[34] Refs. 11 a, b, d. Ref. 6 b, p. 112. Wyckoff, *Am. J. Sci.*, **50**, 317 (1920). W. L. Bragg, *Nature*, **106**, 725 (1921).

[35] Ref. 6e.

[36] Ref. 6f, p. 354.

the compounds, $MgCO_3$,[37] $CaMg(CO_3)_2$,[38] $FeCO_3$[37,38], $MgFe(CO_3)_2$, $Mg2Fe(CO_3)_3$, $MnCO_3$,[37,38] $ZnCO_3$, and $NaNO_3$[38] are without doubt disposed in the same manner as in calcite, while in $SrCO_3$,[36] $BaCO_3$,[36] $BaCa(CO_3)_2$, $PbCO_3$,[36] manganocalcite (RCO_3, in which R represents Mn, Mg, Ca, and a little Fe and KNO_3, the arrangement is like that of aragonite. In the nitrates each sodium or potassium furnishes 1 valence electron, each nitrogen 5, and each oxygen 6, a total of 24 for each "molecule" as in the carbonates. The structures of the various atoms concerned (other than those already given) are: N, $(+7)$ (2×1) (5); Na, $(+11)$ (2×1) (4×2) (1); Mg, $(+12)$ (2×1) (4×2) (2); K, $(+19)$ (2×1) (8×2) (1); Mn, $(+25)$ (2×1) $(5 \times 3 + 3 \times 2)$ (2) or $(+25)$ (2×1) $(1 \times 3 + 5 \times 2)$ (4×2) (2); Fe, $(+26)$ (2×1) $(6 \times 3 + 2 \times 2)$ (2), or $(+26)$ (2×1) $(2 \times 3 + 4 \times 2)$ (4×2) (2); Sr, $(+38)$ (2×1) (6×3) (8×2) (2); Ba, $(+56)$ (2×1) (8×3) (6×2) (8×2) (2); Pb, $(+82)$ (2×1) (8×3) (6×3) (8×3) (6×2) (2), or $(+82)$ (2×1) (8×3) (6×3) (8×2) (6×2) (4×2) (2).

The nitrogen kernel is the same as that of carbon, except for the nuclear charge. The calcium kernel may be replaced by kernels having cubic, tetrahedral,[26] or perhaps (in lead carbonate) octahedral outer shells. The valence pairs around each of the cubic kernels are opposite the 6 faces of the cube. Where the outer kernel shell is a tetrahedron, there is a *kernel* pair opposite (and on the inside of) each face of the *valence* octahedron. If the outer shell of the Pb kernel is an octahedron, the valence pairs are opposite 6 of its 8 faces.

Conclusion.—Enough crystals have probably been considered to demonstrate amply the value of the Lewis theory and the writer's extension of it to the problem of obtaining their *electronic* structures. It has been shown that the valence electrons in these substances tend to form pairs on the center lines between adjacent atoms; also that the number and arrangement of these pairs are in full accord with the atomic structures deduced by Lewis and the author, and the principle (which is at the basis of the author's theory) that the electron groups in an atomic shell tend to lie opposite the faces of the next inner shell. This constitutes very strong evidence in favor of the correctness of these atomic structures and of the theory underlying them.

The further application of these ideas to other crystals, in particular to binary salts (such as sodium chloride), metals and organic compounds, will be given in later papers. It will also be shown how the atomic and electronic structures of many substances can be obtained without the aid of any X-ray measurements whatever.

[37] Wyckoff, Ref. 28.
[38] Ref. 6b, pp. 112–127.

Summary

It has been shown how the Lewis theory of atomic and molecular structures can be applied to crystals whose atomic arrangements have been studied by X-ray means to determine the relative positions of electrons and electron groups. The valence electrons, in the crystals discussed, tend to form complete shells around each atomic kernel, each shell consisting of 4 or 6 electron pairs. Except for elements in the first row of the periodic table, these pairs tend to be opposite the faces of the kernel polyhedra (assuming the atomic structures of Lewis and the writer). The atoms are held together by single bonds, each of which is a valence pair in the shells of 2 atoms (and on or near the centerline between them), or (between the C and O or N and O atoms in the carbonates and nitrates) by double bonds, in each of which there are 2 electron pairs common to 2 atoms. There are lone pairs (pairs not acting as bonds) in arsenic, antimony, bismuth and silicon dioxide (quartz).

The electronic structures of the following crystals are discussed with reference to the foregoing ideas; diamond, silicon, germanium, gray tin, zinc sulfide (cubic and hexagonal forms) cuprous chloride, cuprous bromide, cuprous iodide, silver iodide, (cubic and hexagonal forms), zinc oxide, cadmium sulfide, silicon carbide (carborundum), chalcopyrite $(CuFeS_2)$, pyrite (FeS_2), marcasite (FeS_2), hauerite (MnS_2), iron-nickel sulfide $((Fe\,Ni)S_2)$, arsenoferrite $(FeAs_2)$ loellingite $(FeAs_2)$ smaltite $(CoAs_2)$, safflorite $(CoAs_2)$, cloanthite $(NiAs_2)$, rammelsbergite $(NiAs_2)$, cobaltite $(CoAsS)$, willyamite $(CoSbS)$, gersdorffite $(NiAsS)$, wolfachite $(NiAsS)$, ullmanite $(NiSbS)$, kallilite $(NiBiS)$, arsenopyrite $(FeAsS)$, glaucodotite $(xCoAsS.y$-$FeAsS)$, arsenic, antimony, bismuth, quartz, (SiO_2) calcite, $(CaCO_3)$, aragonite, $(CaCo_3)$, the carbonates $MgCO_3$, $CaMg(CO_3)_2$, $FeCO_3$, Mg-$Fe(CO_3)_2$, $Mg_2Fe(CO_3)_3$, $MnCO_3$, $ZnCO_3$, $SrCO_3$, $BaCO_3$, $BaCa(CO_3)_2$, $PbCO_3$, RCO_3 (manganocalcite), sodium nitrate, and potassium nitrate.

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