# TRANSLATION-GLIDING IN CRYSTALS OF THE NaCl STRUCTURAL TYPE (CONCLUDED)

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## CORRELATION OF TRANSLATION-GLIDING AND STRUCTURE

### THE TRANSLATION-GLIDING DIRECTION

It is well known that crystals of the NaCl type reflect infra-red radiation of certain frequencies exactly as metals reflect ordinary light; these reflected rays are known as residual rays. In order to account for the residual rays according to the electromagnetic theory it is necessary to assume that crystals contain charged particles, which calculations show must be of the order of magnitude of atoms. From this it has been supposed that crystals are built up of charged atoms, or ions, and that the cohesive crystal forces are the attractive forces between the unlike charges of the ions. It is known that the mutual gravitational attraction of particles is not sufficient to account for the experimental strength of crystals, but calculations based on ion attraction give values of about the right order of magnitude.

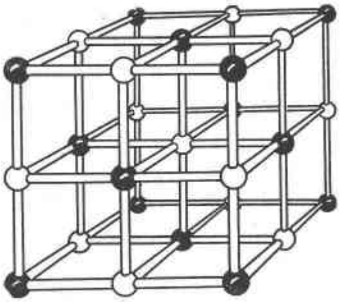

FIG. 7.

A unit cell of the NaCl structural type is shown in figure 7. The translation direction $[1\bar{1}0]$ may be seen to be a unique kind of direction in the structure; it is the direction of densest rows of like ions. Since like ions bear like charges, and unlike ions bear opposite charges, the general significance of the translation direction becomes apparent. For since every ion is exactly like any other of like charge, it is obvious that if any plane of ions containing this row is displaced in the direction of the row by the distance (which may be termed the unit translation-gliding distance) which separates like ions, the original and final configurations of ions, and hence charges, will be identical, and all the properties of the crystal before and after gliding will (ideally) be the same.

While $[1\bar{1}0]$ obviously offers at once the simplest and shortest path for $t$, there are an infinite number of more complicated directions which would give the same result, as far as initial and final states are concerned. For the translation plane (110), the simplest of these other possible translation directions, namely, [010], may be ruled out as electrostatically impossible, for at the mid-translation position, the original configuration of charges across the translation plane would be just reversed, plus for minus and minus for plus. Hence if the normal configuration results in a net attraction across the translation plane, this mid-translation configuration results in a net repulsion of approximately an equal amount. An attempt to produce translation in the direction [010], therefore would be attended by the strongest repulsion, which would prohibit its production. The same kind of reasoning, less rigorously, may be applied to any possible direction in the plane (110), by regarding these planes as composed of alternate rows of plus and minus charges extending in the direction $[1\bar{1}0]$. Normally, a plus row is immediately above a minus row. Translation in the direction $[1\bar{1}0]$ maintains this disposition of rows, as such, unaltered, but translation in any other direction requires a row to occupy a position directly above another of like charge at the mid-translation position, a situation reversing the normal arrangement. Furthermore, any difference in radii of the two kinds of ions composing the structure makes the path $[1\bar{1}0]$ a series of grooves in (110) along which the slipping movement might be expected to be guided.

For the translation plane (001), the following analysis of translation directions will be found useful: For $T=(001)$, all directions have the form $[hk0]$ or the equivalent $[h\bar{k}0]$. When $h+k$ is odd, translation in any of these directions would bring about the following condition: Considering one part of the crystal as fixed, the other as undergoing actual gliding, at half the unit translation distance, every ion in the displaced part occupies a position normally occupied by one of opposite charge. Hence if the normal configuration results in net attraction of the two parts of the crystal across the glide plane (001), the new configuration requires repulsion across that plane by an approximately equal amount. Maximum repulsion, thus, opposes translation by these paths. For a direction in which $h+k$ is even, the same conditions are approached, at some time during translation, and the more closely the more complicated the indices. This leaves the simplest direction of the type when $h+k$ is even, namely $[1\bar{1}0]$, as least opposed to gliding, and hence this becomes the translation direction. Furthermore, any difference in ionic radii of the constituent ions will make $[1\bar{1}0]$ the path requiring least transverse displacement of planes during gliding.

There is a peculiarity about the gliding elements $T=(001)$, $t=[h\bar{k}O]$, where $h+k$ is even, which will subsequently be shown to have a bearing on which plane functions as a glide plane. A glide of half the unit translation-gliding distance in any of these directions (in actual performance, $[1\bar{1}0]$ alone need be considered) brings about an arrangement of charges such that every charge on one side of the glide plane is equally distant and symmetrically placed with respect to an equal number of like and unlike charges across the glide plane, and there is thus on cohesion across the glide plane in the mid-translation position.

## THE TRANSLATION-GLIDING PLANE

Galena and altaite glide only along cube planes while the other crystals glide along both cube and dodecahedron planes, or with very marked preference to gliding along dodecahedron planes alone. For a series of crystals of identical structural arrangement, this behavior seems, at first sight, truly remarkable.

It might be supposed that crystals composed of divalent ions might glide differently than those composed of monovalent ions, and that this might possibly account for the unique behavior of galena and altaite. But the ion charge is, of itself, ruled out of consideration since the divalent-ion periclase glides in quite the same manner as do the monovalent ion alkali halcids, and not as galena and altaite.

The size of the unit cell can, of itself, have no effect upon the glide-plane since a change in scale necessarily changes all distances, and hence coulomb forces, proportionally. This is easily confirmed by preparing a correlation table between unit cell size and glide planes. The table indicates lack of correlation.

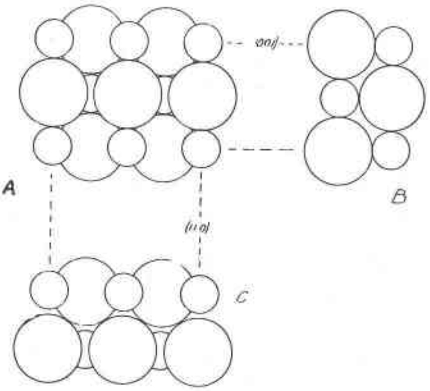

FIG. 8. NaCl structural type, as seen looking along translation-gliding direction [1$\bar{1}$0].

A. Normal ionic configuration.

B. Configuration at half unit translation-gliding distance, with $T=(110)$.

C. Configuration at half unit translation-gliding distance, with $T=(001)$.

Variation in ease of gliding along different planes might supposedly be ascribed to varying smoothness of these planes and thus be related to the ratio of the radii of constituent ions. This can best be illustrated by viewing the structure along the translation direction [1$\bar{1}$0] (figure 8*A*). Then all possible planes, *T*, appear as traces. In the figure, the ion radii are to scale for MgO. Considering, for the first approximation, that the ion radii remain sensibly constant during gliding, it can be seen from figures 8*B* and 8*C* that gliding along either (110) or (001), respectively, involves lifting the plane as well as pushing it. The amount of lift, and thus a measure of the "roughness" of the planes can be calculated.

The amount of lift in gliding along (001) is a function of the ion radius ratio up to a certain ratio beyond which there is no lift. Figure 9 shows that in order that the lift be zero, there must

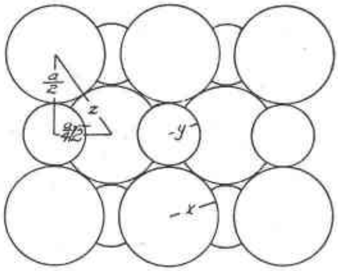

FIG. 9.

be no overlap of the larger ions in their normal positions as seen along $[1\bar{1}0]$. That is,

$$z \geqq 2x, \text{ where } x \text{ is the radius of the larger ion.} \tag{1}$$

From the geometry of the NaCl arrangement (fig. 9),

$$z = \sqrt{\left(\frac{a_0\sqrt{2}}{4}\right)^2 + \left(\frac{a_0}{2}\right)^2} \quad \text{where } a_0 \text{ is the length of a side of the unit cell,} \tag{2}$$

or, simplifying,

$$z = a_0\sqrt{\frac{3}{8}}. \tag{3}$$

Substituting the value of $z$ given by (1),

$$2x \leqq a_0\sqrt{\frac{3}{8}}, \tag{4}$$

or,

$$x \leqq \frac{a_0}{2}\sqrt{\frac{3}{8}}. \tag{5}$$

Now, the radii of the ions are not independent of each other but, if the radius of the larger is designated by $x$, and the smaller by $y$,

$$x + y = \frac{a_0}{2} \tag{6}$$

or,

$$y = \frac{a_0}{2} - x\,. \tag{7}$$

Substituting the value of $x$ given by (5),

$$y \geqq \frac{a_0}{2} - \frac{a_0}{2}\sqrt{\frac{3}{8}}. \tag{8}$$

Dividing (8) by (5)

$$\frac{y}{x} \geqq \frac{\dfrac{a_0}{2} - \dfrac{a_0}{2}\sqrt{\dfrac{3}{8}}}{\dfrac{a_0}{2}\sqrt{\dfrac{3}{8}}} \tag{9}$$

or, numerically,

$$\frac{y}{x} \geqq 0.63.$$

That is, above an ion radius ratio of 0.63 the (001) planes require no lift for translation in the direction $t = [1\bar{1}0]$. Below this ratio, an increasing lift is required along cube planes, down to a value of $x=\frac{a_0\sqrt{2}}{4}$, which corresponds to cubic close packing[22] for the larger ions (figure 10). The maximum separation of (001) planes during gliding is then $\frac{a_0}{4}\sqrt{6}$. The normal separation is $a_0/2$. Thus the lift is

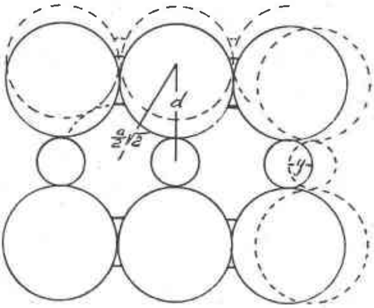

FIG. 10.

$$\text{maximum lift (001)} = \frac{a_0\sqrt{6}}{4} - \frac{a_0}{2} = 0.112a_0.$$

For gliding on (110) the maximum separation may be seen from figure 8*B* to be equal to the sum of the radii of the larger and smaller ions, which is therefore constant, and equal to $a_0/2$. Figure 10 shows the constant lift to be equal to the radius $y$.

$$\text{Lift (110)} = y \qquad (10)$$

$$= \frac{a_0}{2} - x \quad \text{from (7)} \qquad (11)$$

$$= \frac{a_0}{2} - \frac{a_0\sqrt{2}}{4} \qquad (12)$$

$$= 0.147a_0.$$

That is to say, the lift required for translation along (110) is always constant and equal to $0.147a_0$; the lift required along (001) varies with the ion radius ratio. For all ratios, however, the lift in gliding along (001) is less than for (110), and is zero for values of the radius ratio greater than 0.63.

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[22] Below this ratio, the NaCl type of structure is impossible.

Since lift is more or less analogous to friction, it might be supposed that all crystals having an ion radius ratio above 0.63 would glide on cube planes, while those having low ratios might glide on both cube and dodecahedron planes. For this purpose the following correlation table was prepared, using Goldschmidt's[23] values of ion radii:

| CRYSTAL | RADIUS OF CATION | RADIUS OF ANION | $\left(\frac{\text{RADIUS OF CATION}}{\text{RADIUS OF ANION}}\right)$ | TRANSLATION PLANES | |
|---|---|---|---|---|---|
| RbCl | 1.49 | 1.81 | .823 | (110) | ? |
| PbS | 1.32 | 1.74 | .759 | — | (001) |
| NaF | 0.98 | 1.33 | .737 | (110) | (001) |
| KCl | 1.33 | 1.81 | .735 | (110) | (001) |
| KBr | 1.33 | 1.96 | .678 | (110) | (001) |
| PbTe | 1.32 | 2.03 | .650 | — | (001) |
| $NH_4I$ | 1.43 | 2.20 | .650 | (110) | ? |
| Theoretical smooth plane ratio 0.63 | | | | | |
| KI | 1.33 | 2.20 | .604 | (110) | (001) |
| MgO | 0.78 | 1.32 | .591 | (110) | ? |
| NaCl | 0.98 | 1.81 | .541 | (110) | (001) |
| NaBr | 0.98 | 1.96 | .500 | (110) | (001) |
| NaI | 0.98 | 2.20 | .445 | (110) | (001) |

The table brings out the fact that while crystals known to glide only on (001) fall above the smooth-plane ion ratio 0.63, obviously this supposedly critical ratio does not separate crystals which glide on (110) and (001) from those which glide only on (001) and hence has, *of itself*, no particular significance, and ease of gliding on (001) as against ease of gliding on (110) shows no correlation with ion radius ratio.

In an attempt to obtain a hint at what lays at the bottom of this difference in gliding behavior of different crystals built on the same plan and differing only in the kinds of ions in their constitution, the obvious course is to correlate all sorts of ion properties against gliding behavior. Correlation tables, therefore, were prepared, and it was found that the only fundamental ion property which showed

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[23] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente VII, Die Gesetze der Krystallochemie. *Skrifter utgitt av Det Norske Videnskaps-Akademi i. Oslo, I. Mat.-Nat. Klasse,* **1926,** *No.* 2.

any regular and gradational correlation was that of polarizability. Following are the polarizabilities of the ions concerned.[24]

| Cations | | Anions | |
|---|---|---|---|
| $Pb^{++}$ | $3.1 \times 10^{-24}$ cm.$^3$ | $Te^{--}$ | $9.6 \times 10^{-24}$ cm.$^3$ |
| $Rb^{+}$ | 1.81 " | $S^{--}$ | 7.25 " |
| $K^{+}$ | 0.85 " | $I^{-}$ | 6.28 " |
| $Na^{+}$ | 0.21 " | $Br^{-}$ | 4.17 " |
| $Mg^{++}$ | 0.12 " | $O^{--}$ | 3.1 " |
| | | $Cl^{-}$ | 3.05 " |
| | | $F^{-}$ | 0.99 " |

It is immediately apparent from the table that crystals which glide only on (001), *i.e.*, altaite and galena, are composed of anions which head the list and of cations which head the list. Crystals which glide practically only along (110), *i.e.*, periclase, NaF and NaCl, are composed of ions which foot the lists. Crystals which glide along both (001) and (110) with nearly equal ease, *i.e.*, the sodium and potassium bromides and iodides, are composed of ions of intermediate positions in the lists. The correlation is brought out somewhat more forceably by the following table, in which the sums of the polarizabilities of the cations and the polarizabilities of the anions are compared with the planes of gliding. The table prepared in this fashion tends to show that *both* ions have a share in conditioning the gliding plane and the gliding ease.

| Crystal | Sum of Polarizability of Both Ions | Glide Planes | | |
|---|---|---|---|---|
| PbTe | $12.7 \times 10^{-24}$ cm.$^3$ | (001) | ↑ Increasing ease of gliding on (001) and increasing general plasticity | ↓ Increasing *relative* ease of gliding on (110) and decreasing general plasticity. |
| PbS | 10.3 " | (001) | | |
| KI | 7.13 " | (001) and (110) | | |
| NaI | 6.49 " | (001) and (110) | | |
| KBr | 5.02 " | (001) and (110) | | |
| RbCl | 4.86 " | ?[a] and (110) | | |
| NaBr | 4.38 " | (001) and (110) | | |
| KCl | 3.90 " | (001) and (110) | | |
| NaCl | 3.26 " | practically only (110) | | |
| MgO | 3.2 " | practically only (110) | | |
| NaF | 1.20 " | practically only (110) | | |

[a] Data for gliding on (100) is not available for RbCl.

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[24] From *Handbuch der Physik*, Volume **24**, *Berlin*, 1927, p. 449.

The value for doubly negative lead was not available but the approximate value was kindly supplied by Dr. B. E. Warren, of the Department of Physics, Massachusetts Institute of Technology, who had occasion to calculate it for other purposes

The correlation shown in the table is conspicuously in harmony with the experimental results. Thus, haloid for haloid, the potassium salt precedes the sodium salt, and for either series, the sequence runs: iodide, bromide, chloride, fluoride, in harmony with the experimental data collected.

Once the correlation between gliding and polarizability is established, it is not difficult to find the explanation. An electric field has a tendency to separate the positive nucleus from the negative electron shell of an ion. Polorizability is the electric moment thus set up in the ion due to a unit homogeneous electrostatic field. Since this property will not be dealt with mathematically,[25] it will be sufficient to explain its influence on the present problem as follows: If two like ions are separated from one another, they will repel each other less if their polarizabilities are high, and more so if their polarizabilities are low. The property of polarizability increases the attraction and decreases repulsion between ions as usually calculated.

Now it has already been demonstrated that the cube plane is smoother under all conditions than the dodecahedron plane, and that it is very smooth indeed above an ion radius ratio of 0.63. It has already been noted, also, that in gliding along cube planes, a position is approached, halfway along the unit gliding distance, where every ion is just as near a like ion on the other side of the translation plane, as it is to a corresponding unlike ion. Assuming unpolarizable ions, there is no attraction across the plane in this condition, and one part of the crystal could be lifted away from the other without expenditure of any energy. Thus, the maximum amount of work would be done by gliding along this plane, and, since the unit gliding distance is the same regardless of the gliding plane, the average maximum repulsion must be overcome.

When polarizability is taken into account, it is obvious that at the mid-gliding position on (001), the attraction of unlike ions is increased and the repulsion of like ions diminished, depending in amount on the polarizabilities of both ions involved. Thus in gliding to the mid-point of the unit gliding position on (001) the planes retain cohesion and the maximum work or maximum average force is no longer required, and the plane of gliding then becomes dependent on polarizability and smoothness. Since the glide plane depends on the attitude of the load, the cube plane of an NaCl-like

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[25] However see writer's note at end.

crystal composed of strongly polarizable ions becomes at least a possible glide plane. When, as is doubtless the case with altaite and galena, the strong polarizabilities of the ions offer a path of relatively little resistance along (001), gliding takes place along this very smooth plane. If the polarizabilities of the ions are very low, as in NaF, especially directed pressure is necessary to show any trace of gliding along (001), and the crystal glides, by preference, along (110) under a random load, and even then with difficulty due to the roughness of this plane. Not only the preferred plane of gliding, but also the ease of gliding is thus dependent upon the polarizabilities of the ions.

## THE TARICCO FIGURE ON GALENA

The unusual set of gliding elements displayed by galena in the production of Taricco's figure occur under circumstances which are likewise unusual. As a rule, a glide plane extends completely across a crystal. Under such conditions a forced glide in the NaCl structure along (100) in the direction $[00\bar{1}]$, could it be accomplished, would, at half the unit gliding distance, replace plus by minus charges, and *vise versa*, on one side of the glide plane, and a repulsion approximately equal[26] to the normal attraction across (100) planes would result along the active glide plane; consequently cleavage would ensue.

Under the conditions of the Taricco figure, instead of a single plane gliding alone, a prism surrounded by four planes glides. Thus the repulsion across the (100) glide plane is equal and opposite to that across the $(\bar{1}00)$ glide plane, and since the structure of the shell surrounding the prism completely encloses it, cleavage can not ensue. The cross section area of the shell, of course, is enormous compared with that of the gliding surface of the prism, so the surrounding shell can not fail by cleavage.

Still, this figure is unknown for the NaCl-like alkali halcids. If an attempt is made to produce a Taricco figure on any of them, a quite different figure results which has been subject to considerable exposition by Mügge.[27] Radiating from the needle, four parting clefts, (110) and $(1\bar{1}0)$ appear. Between each pair of cracks, a portion of the crystal is displaced away from the needle and upward;

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[26] Assuming rigid spherical ions lacking polarizability.

[27] O. Mügge, Ueber Translationen und verwandte Erscheinungen in Krystallen: *Neues Jahrb.*, **1898**, I, pp. 138–145.

translation-gliding has taken place along $(10\bar{1})$, $(011)$, $(\bar{1}1\bar{1})$, $(0\bar{1}\bar{1})$ in the usual translation direction.

The explanation of the difference is again probably to be found in polarizability. It would appear that the component ions of galena are so polarizable that the repulsion normally to be expected with translation in the direction $[00\bar{1}]$ on $(100)$ is so largely mitigated that this mode of gliding is even easier than in the direction $[101]$ on $(10\bar{1})$.

## CONCLUSIONS

### Conclusions Regarding NaCl-like Crystals

The findings may be briefly summarized as follows: For crystals of the NaCl-like structure, the translation direction, *t*, is determined by the densest rows of like-charged ions. The translation plane, *T*, is a function both of ion radius ratio and of the polarizabilities of the constituent ions. Translation along (001) is associated with high polarizabilities, translation along (110) with low polarizabilities; with intermediate values both (001) and (110) may function as translation-gliding planes under favorable conditions of load.

It is interesting to observe that the translation-gliding direction is identical with the unit translation as used in the geometrical crystal structure theory, provided the original lattice coordinates are retained. The coordinates in practical use have been chosen in such a way as to display the cubic symmetries. Retaining original coordinates, the translation direction, unit translation, direction of closest equivalent lattice points, and thus direction of closest like charges, are identical.

### Extension of Correlation to Other Crystals

At the time of carrying on the research above detailed, the following crystals were known to the writer for which there were available both sufficiently critical translation-gliding and structural data to permit of correlations: salamomniac and low-$NH_4Br$; fluorite; magnesite, siderite, rhodochrosite and smithsonite; dolomite; barite; and anhydrite. For all of these, correlations proved a relation of gliding to structure similar to that found in the NaCl-like crystals, with minor modifications. Thus the translation direction is that of alignment of nearest like charges, but the points occupied by the like charges need not necessarily be equivalent, nor need the line of charges be necessarily truly straight, but may be very slightly zig-zig, etc.

Also, when the original research was carried out, the following crystals were known to the writer for which the structural and gliding data, while not complete, were of such a character as to permit of partial[28] correlation: chalcopyrite, ice, brucite, molybdenite, and graphite. Each of these crystals fitted into the scheme already proposed.

## CONCLUSION OF A GENERAL NATURE

In the foregoing discussions of twenty-seven different crystal species, the fact stands out clearly that the translation direction is specific for a given structural arrangement. However crystals of the same structural arrangement may otherwise differ from one another in properties, they all have the same translation direction in common. In analyzing the various structures for the cause of this uniqueness, it has been pointed out that in each case the translation direction has the structural character of alignment of closest like leptons for all leptons (considered at the same time) in the structure. An adequate mechanistic explanation of the gliding direction has been presented on the assumption that the leptons are individually charged, and thus have the characters of ions, an assumption which easily follows from electrochemical considerations and which has been used to advantage in explaining residual rays and the cohesive forces in crystals.

Two portions of a crystal may relinquish their mutual, normal configuration upon application of sufficient stress, and regain a new, but equivalent, normal configuration provided the alteration pursues a path which allows them to retain cohesion. If cohesion is electrostatically conditioned, so also is translation-gliding, which implies continued cohesion. Of the numerous paths which translation might conceivably take to restore the original configuration of the crystal, one offers a minimum resistance, or, what amounts to the same thing, a minimum loss of cohesion, and this becomes the actual translation direction. For all available data, this unique path has been shown to be connected with paths of closest like-ions, assuming the leptons to be ions, and other paths have been shown

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[28] Thus, in crystals, for which $T$ is known, but $t$ unknown except that it exists as three equivalent directions in $T$, the correlation was regarded as established if the three theoretical directions, $t$, determined a theoretical $T$ which was identical with the actual $T$.

to be impossible. This may be regarded as a substantiation of, and independent evidence for, the theory of the existence of ions in crystals, though not necessarily a proof of it. The successful correlations also have the nature of a partial check on the correctness of the crystal structures considered.

WRITER'S NOTE: This paper was presented in May, 1929, before an informal gathering of Harvard and Massachusetts Institute of Technology physicists and mineralogists interested in crystal structure. At that time, Dr. Hans Müller, Assistant Professor of Physics at the Massachusetts Institute of Technology, evinced a considerable interest in the relation between gliding and polarizability. He informed the writer that this relation would be amenable to a mathematical demonstration. Since then, Dr. Müller has investigated the subject from this viewpoint, and the results of his study, bearing out the writer's correlations in very exact form, will appear in an early number of this Journal.

# NOTES AND NEWS

## EUHEDRAL MAGNESITE CRYSTALS FROM WINKLER COUNTY, TEXAS

JOHN T. LONSDALE, *A. & M. College of Texas.*

The magnesite crystals described in this paper were obtained from drill cores from wells of the Southern Crude Oil Purchasing Company. Most of the material studied came from the company's Well 89-E-1, located 2310 feet from the east line and 330 feet from the north line of Section 40, Block B-5, Winkler County, Texas. Additional specimens came from a nearby well the exact location of which is not known. The core from Well 89-E-1 was taken at 2690 feet, the formation being Permian and known as the "white lime". The core from the nearby well is believed to have been taken at a level several hundred feet higher, from the "brown lime", a higher Permian formation. The specimens were submitted to the writer by A. L. Ackers and E. M. Hawtof of the geological staff of the company.

Euhedral magnesite crystals are not common. Austin F. Rogers has described crystals from San Jose, California, and Lillian M. Dobbel crystals from Orangedale, Nova Scotia.[1] There are only a few additional occurrences of crystals from the whole world and textbooks of mineralogy contain very few data on the crystallography of the mineral. The rarity of the crystals and the fact that those from Winkler County are different crystallographically from the other North American occurrences accounts for the present note.

The magnesite crystals occur disseminated through fragments of the well cores mentioned above. They appear much as phenocrysts in an aphanitic igneous rock. The matrix is a dolomitic limestone containing chert or flint nodules. Many of the magnesite crystals are stained with petroleum or asphalt. The crystals have originated by replacement of the dolomite by magnesium bearing solutions.

The crystals measure from about 1 mm. up to about 5 mm. in length. They

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[1] Rogers, Austin F., Euhedral Magnesite Crystals from San Jose, California: *American Mineralogist*, Vol. **8**, pp. 138–140, 1923. Dobbel, Lillian M., Magnesite Crystals from Orangedale, Nova Scotia: *American Mineralogist*, Vol. **8**, pp. 223–228, 1923.