

*On the presentation of chemical analyses of minerals.*

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THE results of a chemical analysis of a mineral are always presented, in the first place, as percentages of elements or oxides present,<sup>1</sup> and until recently the only possible further treatment of these values was to calculate atomic or molecular ratios, group them according to accepted isomorphous groups, and deduce (if possible) an integral chemical formula. The degree of approximation to integral ratios accepted as satisfactory is, of course, quite arbitrary, and a decision as to the degree of complication acceptable in a chemical formula has often had to rest on very inadequate evidence. Some workers prefer to adjust the final ratios to show the errors evenly distributed, a procedure which has no real advantages.

The introduction of X-ray methods of structure analysis, and the measurement of the actual sizes of the structural units of many minerals, has opened the way to much more significant methods for the presentation of chemical analyses, and there is now rarely any justification for guesswork in the assigning of a chemical formula. Unfortunately, the possibilities and the limitations of a presentation based on structural data are not always realized and it is the purpose of this note to call attention to some points in this connexion.

Wherever an accurate determination of the density and unit-cell size of the mineral has been made on the actual material analysed, the most satisfactory presentation of a chemical analysis is in atoms, ions, or molecules per unit cell of the several constituents shown by the analysis;

<sup>1</sup> Often, most of the oxides shown in an analysis were actually weighed as such. This has one advantage not often realized; it is not necessary to know the atomic weights used by the analyst in order to make use of the analysis. This may seem unimportant, but is not always so; thus in any analysis of an antimony mineral, Sb will probably be reported as the element after weighing as  $Sb_2S_3$ , and the percentage Sb reported will be appreciably different according as 120.2 or 121.76 is used as the atomic weight of Sb. A note on the weighing-forms and atomic weights employed is certainly desirable in any analysis having claims to high accuracy.

these may be styled empirical unit-cell contents as distinct from those 'unit-cell contents' referred to below, which are really atomic ratios to a more or less arbitrary basis. Such a presentation involves no assumptions whatever, and carries the greatest possible conviction, especially when a new chemical formula is being proposed. It has one disadvantage, that the accumulated errors of the density and X-ray measurements are applied to the chemical data, but this cannot be regarded as serious. There are, however, certain limitations to its use, and certain precautions necessary if it is to be used to full advantage, not always recognized.

If the analysis shows any impurities, their nature should be ascertained and the density corrected accordingly,<sup>1</sup> if possible; if the density cannot be accurately corrected for the impurities, it will at least be possible in almost every case to assign limits to the probable true density. It is not necessary to recalculate the analysis to 100%, whether impurities are present or not; a more convenient procedure is to compute the atomic or molecular ratios,  $P/M$ , for each constituent<sup>2</sup> by division of its percentage,  $P$ , in the mineral by its molecular weight,  $M$ , and then find a conversion factor  $F$  by which to multiply the atomic ratios to give cell contents  $FP/M$  directly; if the cell volume is  $V$  and the density (corrected for any impurities)  $D$ , then  $F = VD/1.649S$ , where  $S$  is the net summation of the analysis after subtraction of impurities.<sup>3</sup> Further, the probable percentage error in  $F$  should be calculated from the known or assessed probable errors in the cell sides and density. This is relatively simple and can nearly always be effected, but probable errors in the chemical analysis are much more difficult to assess; the accuracy attainable in chemical analyses has been discussed by W. F. Hillebrand and G. E. F. Lundell<sup>4</sup> and by E. S. Larsen,<sup>5</sup> and it is evident that where any

<sup>1</sup> Where the impurity is adsorbed water, it is not really certain what density should be assumed for the water; however, a value of 1 is not likely to introduce appreciable error.

<sup>2</sup> Most mineral analyses are primarily presented in a mixed form, mainly as oxides, but with some negative ions (F', Cl', S'), and 'less O for' these latter. To deduce the atomic ratio for oxygen a formal calculation of the percentage of oxygen is unnecessary; the molecular ratios of the several oxides are multiplied by the number of oxygen atoms in each oxide added, and the atomic ratio for any oxygen subtracted 'for F', Cl', &c.' subtracted from the sum.

<sup>3</sup> These relations may seem too obvious to require stating, but instances could be cited from the recent literature where corrections for impurities have been wholly neglected and conversations have shown that the way in which a correction may be effected is often not understood.

<sup>4</sup> W. F. Hillebrand and G. E. F. Lundell, Applied inorganic analysis. New York, 1929.

<sup>5</sup> E. S. Larsen, Amer. Journ. Sci., 1938, ser. 5, vol. 35, p. 94. [M.A. 7-183.]

unusual type of isomorphous substitution is postulated the magnitude and effect of possible errors in the analysis should receive especial consideration.

As a general rule, the calculation of empirical unit-cell contents shows that the several kinds of atoms present, when divided into groups on well-established lines, add up to integral numbers (within the limits of the probable errors of the chemical analyses, and of the cell-side and density determinations<sup>1</sup>) and can be assigned to the several lattice positions of the crystal-structure; but it must not be assumed that this will necessarily be the case, and that a failure to attain integral relations indicates an inaccurate analysis. Recent work has shown that vacant lattice positions are comparatively frequent, and the possibility of an excess must not be disregarded, though in general an excess probably indicates an error.

By far the most troublesome constituent of minerals for the satisfactory presentation of a chemical analysis is water, since it may be present adsorbed, when it constitutes an impurity, or as hydroxyl groups, or as molecular water of crystallization, and the accurate distinction of the three forms is rarely possible. As a general rule, small quantities of water lost at a low temperature may be assumed to be adsorbed, but the distribution of water into impurity and constitutional (including water of crystallization) is often essentially arbitrary and constitutes the most serious weakness in the determination of empirical cell contents.

The effect of adsorbed water, not recognized as an impurity, on the calculated cell contents deserves special consideration since it is one of the most difficult of all impurities to detect, even when present to the extent of several per cent. The observed density will be low, but the oxygen atoms per unit cell (including the oxygen of the water) will usually be high,<sup>2</sup> and the other atomic contents low. Now in a large proportion of minerals the oxygen atoms (or more generally, O", OH', and F' ions) are the largest atoms present and there is no room for an

<sup>1</sup> It must, of course, be remembered that these last, affecting the factor  $F$ , will necessarily affect all constituents equally or in the same direction, and cannot affect their distribution.

<sup>2</sup> The low density makes the factor  $F$  low, but because water contains a larger percentage of oxygen than any other compound the oxygen percentage will be high, and as a general rule the latter effect will preponderate; as an illustration we may calculate the effect of 1 per cent. adsorbed water on the apparent cell contents of quartz and of litharge: Si 2.951, O 6.002, H 0.199 (in place of Si 3, O 6); Pb 1.962, O 2.208, H 0.491 (in place of Pb 2, O 2); the effect is, of course, more marked the smaller the percentage of oxygen in the substance.

excess of them; hence if the oxygen atoms per unit cell appear to exceed the most probable integral value by more than the probable error of the factor  $F$ , adsorbed water may usually be suspected—to prove it is another matter.

In minerals containing much constitutional water (hydroxyl or water of crystallization), and especially in deliquescent or efflorescent salts, the uncertainty of the water content makes the calculation of reliable unit-cell contents difficult or impossible; the same difficulty may arise with certain iron minerals which are not readily opened up (such as staurolite), when the uncertainty as to the division of the total iron into ferrous and ferric renders the total oxygen content uncertain. In such cases it may be preferable to have recourse to one of the several presentations based on an assumption. Such forms of calculation are also valuable for presentation of numbers of analyses from the literature (for few of which correlated density and X-ray data are likely to be available), or when for any reason adequate accuracy in the X-ray or density data is not attainable.

The first essentials in all presentations based on an assumption are that the basic assumption should be clearly and explicitly recognized, should be carefully selected to suit the particular circumstances, and that there should be adequate evidence in justification of it. Such evidence of justification will normally take the form of analyses with correlated density and X-ray data, from which empirical unit-cell contents supporting the proposed assumption are calculated. Or it may be shown that the compound in question is isomorphous with another for which the validity of the proposed assumption has been demonstrated, and that there is reason to believe the extension justified. Or the assumption may be that X-ray (or more rarely, density) measurements made on a sample other than the actual sample analysed<sup>1</sup> are accurate enough for use in the calculation of the analysis, when evidence is desirable that the cell-sides (or density) of the species in question do not vary appreciably, or that they vary in regular manner, so that the values for the sample analysed may be fairly deduced from its composition.

When X-ray or density data, or both, are lacking or inaccurate it is no longer possible to calculate the empirical cell contents. But since the number of lattice positions available for any atom or group of atoms in a crystal-structure is always integral, and since in many cases all, and in

<sup>1</sup> It is most unscientific for chemical analysis and optical, X-ray, or other physical data to be made on separate samples without explicit statement of the fact, and a careful check of the uniformity of the material studied is always desirable.

almost every instance some group or groups of lattice positions are exactly occupied,<sup>1</sup> without excess or defect (within the accuracy of experiment), it is often justifiable to assume that the unit-cell contents of the specimen analysed will show an integral value for some atom or group of atoms,<sup>2</sup> and to calculate atomic, molecular, or ionic ratios on this basis; such ratios are often wrongly called unit-cell contents, but they are really no more than atomic ratios to an arbitrary basis, and should always be so described, specifying the basis assumed.

The most suitable basis to use for presentation will vary, not only with the type of mineral under examination, but also with the purpose of the presentation; thus to provide convincing evidence of an unusual isomorphous substitution, that basis of calculation should be selected which reduces the substitution to be proved to a minimum, so that any other basis of calculation gives a greater apparent degree of substitution.<sup>3</sup> The principal types of minerals for the present purpose are: (i) those whose analyses which are usually reported mainly or wholly in terms of oxides, whose largest ions are O<sup>''</sup>, OH<sup>'</sup>, and F<sup>'</sup>, and in which it is not possible to select groups of constituents, failure of which to balance necessarily indicates an inaccurate analysis; (ii) minerals whose analyses are usually reported in terms of ions, which must necessarily balance in an accurate analysis—for example, halides;<sup>4</sup> (iii) 'atomic' minerals, whose analyses are reported in terms of atoms, such as sulphides and selenides, but which differ from the formally similar ionic minerals in that there is often no exact balance (as in the well-known case of pyrrhotine). There are some broad distinctions as to the most suitable basis of calculation for each of these types, though each individual case must be considered on its own merits.

Among minerals normally reported in terms of ions the fact that

<sup>1</sup> The electrical conductivity of some ionic crystals which show no excess of either component is probably due to vacant positions in both anion and cation lattices; proof of this suggestion appears to be still incomplete, and the proportion of vacancies called for is very small (up to 0.02 per cent. in calcite).

<sup>2</sup> The actual integer to be accepted may be decided on the basis of approximate unit-cell contents, based on an approximate density and cell-sides, or by extension from an isomorphous or isostructural compound.

<sup>3</sup> Thus in evidence of the substitution of C for Ca in carbonate-apatites, it was shown that no basis of calculation of the analyses could be found requiring less of this substitution than 0.2 atom per unit cell. (This vol., p. 400.)

<sup>4</sup> Recent work has shown that even so typically ionic a mineral as rock-salt may contain an excess of sodium ions, balanced only by free electrons; such excess is usually far less than the probable accuracy of the majority of analyses, but clearly an ionic balance need not always be quite exact.

positive and negative ions must balance may be used to classify analyses as to their probable accuracy, and the most suitable basis of calculation will normally be to give an integral value to the sum of all the ionic charges<sup>1</sup> ( $\Sigma(\text{ionic charge}) = \text{const.}$ ), but occasionally other bases may be preferable. The same method may be used in salts which are normally reported in terms of oxides, such as sulphates, if there is definite evidence that the salt has an ionic structure and is not contaminated with any acidic or basic impurity. With hydrated salts, it will generally be preferable to exclude the water from the sum to which an integral value is assigned, since it is the component most likely to be affected by analytical error; departure of the water content from an integral ratio may then indicate either impurity, an inaccurate analysis, or that the hydrate is of the zeolitic type.

In minerals such as sulphides and selenides, where vacant lattice positions are very common, it is generally best to assume that one group of atoms (metal or sulphur, &c.) occupy an integral number of lattice positions and the other group have vacant positions; but the possibility of extra interstitial atoms, or of the replacement of sulphur atoms by sulphur pairs in some structures,<sup>2</sup> must not be ruled out without direct proof. Among these minerals it is generally impossible to discuss the probable accuracy of an analysis on internal evidence, which is especially unfortunate, as many analyses of sulphide minerals are of doubtful accuracy.

Among silicates and other minerals which are normally reported in terms of oxides, the majority of structures show great possibilities of isomorphous substitution, but in most cases it is justifiable to assume that the sum of the large ions,  $O'' + OH' + F'$ , will be integral and to use this as a basis of calculation ( $\Sigma(O'' + OH' + F') = \text{const.}$ ). For anhydrous minerals this usually is a simple matter,<sup>3</sup> and where the water can be

<sup>1</sup> The possibility that an ion may be replaced by one of a different charge without the creation of a lattice vacancy must not, however, be forgotten; neutrality could be maintained by interstitially accommodated ions or by a simultaneous parallel substitution among the ions of opposite sign.

<sup>2</sup> Another possibility is that sulphur atoms may enter some of the metal positions, or vice versa. In any particular sulphide or similar mineral, calculations to an assumed basis can do no more than demonstrate variability and departure from a constant simple metal-sulphur ratio; the manner of this variation can only be profitably discussed on a basis of empirical cell contents, at least in the present state of our knowledge of such structures.

<sup>3</sup> The exception is with minerals where the determination of the state of oxidation of such elements as Fe, Mn, or V is liable to be inaccurate from the nature of the mineral (e.g. staurolite). For such minerals  $\Sigma(\text{cations}) = \text{const.}$  will often be a more satisfactory mode of presentation.

shown to be wholly water of crystallization, as in zeolites, it is best to exclude it from the oxygen sum, but hydrous silicates including both hydroxyl and water of crystallization give rise to more serious problems owing to the possibility that the water positions may be incompletely filled or that there may be appreciable amounts of adsorbed water. In some cases it may be possible to find another satisfactory basis of calculation, but in others, such as the clays, there does not appear to be any really satisfactory basis available. Calculations to an 'anhydrous basis' amount to an additional assumption that the number of hydroxyl groups per unit cell is constant; this is certainly not the case in the micas, and there is no apparent reason why it should be even approximately true in the clays. In general, if  $(O' + OH')$  cannot be accurately determined and there is no evidence that  $OH'$  is likely to remain constant, a really satisfactory basis of presentation of the chemical analysis will rarely be found.

It is possible that a distinction between hydroxyl and water of crystallization or adsorbed water might be obtained by the use of deuterium oxide, since the ease of hydrogen exchange is likely to vary widely with the binding; no experiments appear to have been made as yet in this direction, but we would suggest that it may be found a useful tool in work on hydrous minerals.

When calculations of analyses are made to an assumed integral number of atoms per unit cell of some constituent or group of constituents,  $\Sigma R = K$ , on material for which X-ray data are available, it is usual to calculate the density on the basis of the analysis, X-ray data, and assumed integral number  $K$ ; using the same symbols as above, it is clear that if  $\Sigma(P/M)$  indicates the sum of the atomic ratios  $P/M$  for the several constituents included in the sum  $K$ , the conversion factor  $F = K/\Sigma(P/M)$ , and hence  $D(\text{calc.}) = 1.649SF/V = 1.649SK/V\Sigma(P/M)$ . The probable percentage error in  $D(\text{calc.})$  will be equal to that in  $V$ , plus an unknown amount due to errors in the chemical analysis or to departures from the assumed integral value  $\Sigma R = K$  atoms per unit cell. This value  $D(\text{calc.})$  is of course a calculated density of the pure mineral, and is to be compared with the observed density as corrected for impurities.

In a form of presentation which is occasionally seen, the atomic ratios, except that of oxygen, are first calculated on an assumed value for the total cations per unit cell, and the oxygen ratio is then taken by difference from an assumed value for total anions per unit cell  $(O' + OH' + F')$ , usually; anionic and cationic charges or valencies are then totalled and

compared, and any failure of them to balance<sup>1</sup> is taken to indicate inaccuracy of the chemical analysis or undetected impurities in the material. This mode of presentation has much the same value and applicability as an ordinary calculation to an assumed total number of cations per unit cell. It has the disadvantage that the results are liable to be misunderstood by those not familiar with the method and that it throws the whole of the experimental errors on one constituent, oxygen.

Whatever form of presentation is used, the figures shown will be affected by any inaccuracies in the chemical analyses, which may take three forms: either (i) a constituent may have been accurately separated, but inaccurately determined, when that constituent (and the sum) will be low or high, the other constituents being correct, or a separation may be imperfect, when one constituent will be low and another high by (ii) the same or (iii) a different amount;<sup>2</sup> and (iii) may be formally treated as a combination of (i) and (ii).

In an analysis reported in terms of oxides and presented as empirical unit-cell contents, an error of separation whereby some of an oxide  $A_mO_n$  (of molecular weight  $a$ ) is reported as  $B_pO_q$  (of molecular weight  $b$ ), the calculated oxygen atoms per unit cell will be high if  $am/n < bp/q$ , but beyond this, only the elements A and B actually involved in the separation will be affected. An error of determination, on the other hand, will affect all constituents; if  $x\%$  of the oxide  $A_mO_n$  is lost, all the other constituents will be high by a factor  $(1+x/100)$ ; oxygen may be low or high.<sup>3</sup>

When the analysis is presented as atomic ratios to an assumed basis, analytical errors may have very different effects according to the basis of calculation adopted. Thus if the adopted basis is  $\Sigma(\text{cations}) = \text{const.}$ , an error of separation will affect the calculated density and the ratios for all the constituents equally except oxygen and the two constituents directly involved, the effect being an increase if  $a/m < b/p$  (symbols and

<sup>1</sup> Except in this form of calculation, anionic and cationic charges or valencies must necessarily balance in analyses which are presented mainly in the form of oxides with an oxygen deduction for any ion reported; failure to balance simply indicates mistakes in calculation. In analyses of ionic minerals reported in terms of ions, failure of the positive and negative ions to balance may occur, and indicates inaccuracy of the analysis (lattice defect in the crystal is usually too minute to detect). Analyses of 'atomic' minerals, such as sulphides, rarely balance exactly.

<sup>2</sup> The errors will balance only if both the constituents involved are weighed in the forms they are reported in or have the same conversion factor.

<sup>3</sup> If the several other constituents are denoted by  $B_pO_q$ , their molecular weights by  $b$ , and the percentages present by  $y$ , oxygen will be low if  $\Sigma y(n/am - q/bp)$  is positive.



error as above), while oxygen may be high or low according as this effect or that due to the different oxygen contents of  $A_mO_n$  and  $B_pO_q$  preponderates (the latter effect makes O high if  $am/n < bp/q$ ). An error of determination (deficit) may make the oxygen ratio high or low, according as the number of oxygen atoms per metal atom in the oxide directly affected,  $n/m$ , is less or greater than the mean number in the other oxides; the calculated density also may be high or low, while all other constituents will be high.

If the adopted basis is  $\Sigma(O, OH, F) = \text{const.}$ , an error of separation will make the calculated density and atomic ratios all high if  $am/n < bp/q$ , while a deficit in any determination will make the other constituents all high, but the density may be either high or low.

In the above, errors in the separation and determination of the metallic oxides only have been considered. But the determination of some of the anions, particularly fluorine, and the separation of water into hydroxyl and molecular water are especially liable to error. Errors in the determination of hydrate (including zeolitic) water will not affect any of the other constituents unless calculations are made to a basis including the hydrate water, which is unusual. An error by which water which is really present as hydroxyl is accounted as adsorbed water, or lost, will have similar effects to a deficit in a fluorine (or other anion) determination. The effect of a deficit of  $x\%$  in fluorine or other anion on the empirical unit-cell contents is to make them all high by half the amount by which  $F'$  is low, (so that  $\Sigma(O, OH, F)$  is low by half the amount that  $F'$  is). In a presentation in atomic ratios to the base  $\Sigma(\text{cations}) = \text{const.}$ , a deficit in fluorine will only affect the oxygen ratio and  $\Sigma(O, OH, F)$ , the former being high and the latter low by the factor  $(1 - x/100)$ . If the basis adopted is  $\Sigma(O, OH, F) = \text{const.}$ , a deficit in  $F'$  leads to high values for all the other constituents, especially oxygen, and normally a high calculated density.<sup>1</sup> If hydroxyl water is accounted as hydrate water, the effects will in general be the same, except that the empirical unit-cell contents will not be affected beyond  $O''$  and  $OH'$ , and the calculated densities will be higher than if the water were lost or accounted as adsorbed water.

Errors in the determination of the net state of oxidation of the mineral (commonly a 'ferrous iron' determination)<sup>2</sup> affect the summation, and

<sup>1</sup> The calculated density will be low if the mean equivalent weight of the oxides is less than that of the anion which is in deficit.

<sup>2</sup> It is not always realized that the 'ferrous iron' determination is really no more than a determination of the amount of oxygen necessary to convert all the oxides

hence in a presentation as empirical unit-cell contents, an under-estimation of the degree of oxidation (high value for FeO or  $V_2O_3$ , low value for  $Mn_2O_3$  or  $MnO_2$ ) results in high figures for all the constituents not directly affected. In a presentation to the basis  $\Sigma(O, OH, F) = \text{const.}$ , under-estimation of the degree of oxidation naturally again results in high values for all the other constituents, while with the basis  $\Sigma(\text{cations}) = \text{const.}$  the other constituents are unaffected.

In analyses of the kind that are usually reported as ions or atoms a deficit in determination will make all the other ionic ratios high in a presentation as empirical unit-cell contents or as ionic ratios to a basis  $\Sigma(\text{ionic charge}) = \text{const.}$  An error of separation, in this class of analysis, will involve  $x\%$  of A being reported as  $y\%$  of B, since the weighing-forms are rarely the free elements, and any assessment of the effect of such an error must involve the conversion factors for the weighing-forms adopted. If the analysis is a volumetric one, the errors in A and B will often be in the proportion of their equivalent weights; if then the constituent which is in deficit (A) is the heavier, the net sum will be low, and the other ionic ratios will all be high for a presentation as empirical unit-cell contents, but normal for ionic ratios to a basis  $\Sigma(\text{ionic charge}) = \text{const.}$

Any discussion of the presentation of chemical analyses would be incomplete without some mention of a method formerly general, as an isomorphous mixture of two or more end-members. For an isomorphous mixture of molecular compounds (for example, hexachlor- and hexabrom-benzene), this method is perfectly suited, but very few minerals are molecular compounds, most being ionic, and in the few that are molecular, the molecule and crystal are often coextensive, as in diamond or quartz. For ionic compounds presentation in terms of isomorphous end-members loses any physical significance, and ceases to be of more than formal value (suited for plotting graphs of correlated physical constants and composition) as soon as variations in both ions occur; in silicates (where in many cases the anion is a chain or net structure coextensive with the crystal, and the term molecule loses all

present to that state of oxidation which is stable under the conditions of the determination. The allocation of the whole of the observed reducing power to FeO, or to  $FeO + V_2O_3$ , is often purely an arbitrary assumption, necessary because we have no means at present of detecting and determining other lower oxides such as  $Ti_2O_3$ ,  $UO_2$ , or  $Cu_2O$ , or higher oxides such as  $Mn_2O_3$  or  $Co_2O_3$ , which might conceivably be present. The term 'net state of oxidation' includes, of course, 'available oxygen' determinations in peroxidized minerals such as piedmontite, manganite, or minium.

force) the necessary postulation of numerous 'end-members', incapable of independent existence and of no structural significance, again reduces this method of presentation to a purely formal one suited only to correlation graphs. The fact that all eight pure end-members of an isomorphous mixture  $(\text{NH}_4, \text{K})(\text{Al}, \text{Fe})[(\text{S}, \text{Se})\text{O}_4]_2 \cdot 12\text{H}_2\text{O}$  are known and stable does not dispose of the fact that a representation of the alum as an isomorphous mixture of four of them is purely formal and of no physical significance; the same applies to the spinels, where most of the end-members are known, and far more forcibly to such a group as the tourmalines where few, if any, of the conceivable 'end-members' are known in anything approaching a pure state. Nor does the fact that the existence of certain silicate molecules in melts is probable necessitate the existence of the same molecules in the solid state.

*Summary.*

Wherever the necessary data are available with adequate accuracy, the most satisfactory presentation of a chemical analysis is as empirical unit-cell contents, calculated from the cell-sides, density, and chemical data. When empirical unit-cell contents cannot be calculated, some assumption is necessary for a presentation having claims to any structural significance; the assumption to be made should be carefully chosen and explicitly stated. A number of assumptions suitable in special cases are discussed, as is the technique of calculating empirical unit-cell contents, and the effects of errors in the chemical analysis on the several forms of presentation.

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