THE SALT NORM: A Quantitative Chemical—Mineralogical Characterization of Natural Waters

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ABSTRACT

The new computer program SNORM calculates the salt norm from the chemical composition of a natural water. The salt norm is the quantitative ideal equilibrium assemblage that would crystallize if the water evaporated to dryness at 25°C and 1 bar pressure under atmospheric partial pressure of CO_2. SNORM proportions solute concentrations to achieve charge balance. It quantitatively distributes the 18 acceptable solutes into normative salts that are assigned from 63 possible normative salts to allow only stable associations based on the Gibbs Phase Rule, available free energy values, and observed low-temperature mineral associations.

Although most natural water compositions represent multiple solute origins, results from SNORM identify three major categories: meteoric or weathering waters that are characterized by normative alkali-bearing sulfate and carbonate salts; connate marine-like waters that are chloride-rich with a halite-bischofite-carnallite-kieserite-anhydrite association; and diagenetic waters that are frequently of marine origin but yield normative salts, such as Ca-bearing chlorides (antarcticite and tachyhydrite) and sylvite, which suggest solute alteration by secondary mineral reactions. The solute source or reaction process within each of the above categories is commonly indicated by the presence or absence of diagnostic normative salts and their relative abundance in the normative salt assemblage. For example, salt norms (1) may identify lithologic source; (2) may identify the relative roles of carbonic and sulfuric acid hydrolysis in the evolution of weathering waters; (3) may identify the origin of connate waters from normal marine, hypersaline, or evaporite salt resolution processes; and (4) may distinguish between dolomitization and silicate hydrolysis or exchange for the origin of diagenetic waters.

INTRODUCTION

Chemical composition plays a central role in the classification of natural waters and interpretation of their source and evolution. In this paper we offer a quantitative chemical-mineralogical method of characterizing natural waters that desribes the solutes as an idealized $25^{o}C$ equilibrium assemblage of mineral salts. We suggest that characterization of a water's composition as an assemblage of salts leads to a more detailed chemical classification of natural waters and hopefully provides indications of solute source and subsequent interactions.

Dissolved constituents in natural waters expressed as salt abundances are not new. In the nineteenth century, it was a common practice to report water compositions in terms of abundances of simple salts. As Hem (1970) points out, this practice predated the acceptence of the Arrhenius concept of dissociated ions, and, although it attempted to express water composition in terms of the salts produced upon evaporation, it was actually more closely related to the classical gravimetric analytical procedures than to the natural occurrence of mineral salts. Such schemes relied chiefly on forming simple salts with little regard to salt association. It is not surprising then that this form of expressing water compositions diminished in the twentieth century with only occasional use in the more recent literature (see, for example, Rankama and Sahama, 1950, p. 318; Lambert, 1978).

Comparison and study of both marine and non-marine evaporite deposits have demonstrated some striking differences in the associated salt mineral assemblage (Stewart, 1963; Braitsch, 1971; Jones, 1970; Eugster, 1980; Sonnenfeld, 1984), that commonly are indicative of both lithologic origin and subsequent geochemical evolution of the dissolved constituents (Hardie and Eugster, 1970; Eugster and Hardie, 1978; Eugster and Jones, 1979; Eugster and others, 1980). Thus, it might be informative to attempt reconstruction of the solute content of a natural water into the equilibrium salt assemblage expected were the solution evaporated to dryness under earth surface conditions.

This salt assemblage is analagous to the CIPW norm (Cross and others, 1902), which is an idealized equilibrium assemblage of igneous minerals calculated from the rock's chemical composition. The CIPW norm has proven useful in igneous petrology for characterizing and classifying igneous rocks and providing quantitative data for interpretation of the origin and evolution of an igneous complex. We suggest a parallel application of the idealized equilibrium salt assemblage--the salt norm, which is calculated from a water's chemical composition. Indeed, its similar construction and association permits the general classification of natural solutions based on saline mineral assemblages. Such classifications are more detailed and suggestive of solute origin and subsequent interaction than major cation-anion predominance currently, the most commonly used system of hydrochemical classification.

Transformation of a standard water analysis into the normative salt assemblage is performed by the new computer program SNORM. Preliminary results from SNORM for a wide variety of water compositions suggest that, for example, a few key normative salts are diagnostic of source, such as meteoric as opposed to connate marine waters, and the relative abundance of selected normative salts is indicative of the character of water-rock interaction in subsurface environments, such as silicate hydrolysis in a crystalline host as opposed to dolomitization in a carbonate matrix. Examples of salt norms and their interpretation will be presented and discussed following a description of SNORM.

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THE SNORM PROGRAM

SNORM is a computer program written specifically to compute the normative salt assemblage from the solute concentration data in a conventional water analysis. Although the salt norm can be visualized as the solid residuum that coexists with the small, last vestige of solution upon evaporation at 25°C, the normative assemblage is computed directly from solute concentrations without proceeding along an evaporation path with its myriad succession of brine-solid interactions. Neither brine evolution nor character of the vestigial brine are considered; SNORM only distributes the solutes into the appropriate liquid-free salt assemblage. The program transforms 18 solutes (table 1) into a normative salt assemblage from a listing of 63 possible salts (table 2).

The program is written in FORTRAN IV (Appendix I). The structure of SNORM and a description of the computational procedures are given in Appendix II, user procedures and options in Appendix III, and sample print-outs in Appendix IV. SNORM performs three major tasks: (1) it reads solute concentration values from a conventional water analysis into the program, recasts these values into other appropriate concentration units, and adjusts the solute concentrations to yield cation-anion charge balance; (2) it determines the equilibrium normative salt assemblage based on the principles

Table 1. Solutes in water analyses that SNORM recasts into the normative salt assemblage

CATIONS			ANIONS	
Major				
	Mg^{2+}	Na^{+}	Cl^{-}	HCO_3^{-}
	Ca^{2+}	K^{+}	SO_4^{2-}	CO_3^{2-}
Minor				
	Li^{+}	Sr^{2+}	Fl^{-}	NO_3^{-}
	NH_4^{+}	Ba^{2+}	Br^{-}	B^{*}
			I^{-}	PO_4^{3-}

*Boron assigned as borate with a charge of -7/12 (-0.583) per boron or the charge per boron that is appropriate for the borate stoichiometry of the normative salt in the assemblage.

of phase equilibria, and assigns quantitatively all solutes into the salts of the assemblage; and (3) quantitatively recasts the major-solute normative salts into their respective single cation-single anion simple salts for graphic-classification purposes.

Our approach to accomplish the transition from the first task to the second requires exact cation-anion charge balance among the solutes for distribution into the electrically neutral normative salt assemblage. If an unbalanced population of cation and anion charges were to be distributed, excess charge would remain unassigned or salt compositions would have to be adjusted to form charged salts to compensate for the charge imbalance among the solutes. Both alternatives are undesirable; the former would require deleting the excess residue, and the latter would require each normative salt to contain excess cation or anion to compensate for the charge imbalance among the solutes.

Solutes

The solutes (table 1) that SNORM distributes into normative salts (table 2) were selected to comply with two criteria: (1) The solute, at least occasionally, occurs in natural waters in more than negligible (trace) concentrations; and (2) the solute forms its normative salt(s) through direct

Table 2. Abbreviations of normative salts in SNORM and their chemical formulae

		(Bi)carbonates			
cal	Calcite	$CaCO_3$	kal	Kalicinite	$KHCO_3$
mag	Magnesite	$MgCO_3$	lca	--	Li_2CO_3
dol	Dolomite	$CaMg(CO_3)_2$	tes	Teschemacherite	NH_4HCO_3
tro	Trona	$Na_3H(CO_3)_2\cdot 2H_2O$	str	Strontionite	$SrCO_3$
pir	Pirssonite	$Na_2Ca(CO_3)_2\cdot 2H_2O$	wit	Witherite	$BaCO_3$
		Sulfates			
anh	Anhydrite	$CaSO_4$	blo	Bloedite	$Na_2Mg(SO_4)_2\cdot 4H_2O$
gyp	Gypsum	$CaSO_4\cdot 2H_2O$	leo	Leonite	$K_2Mg(SO_4)_2\cdot 4H_2O$
kie	Kieserite	$MgSO_4\cdot H_2O$	pic	Picromerite	$K_2Mg(SO_2)_2\cdot 6H_2O$
eps	Epsomite	$MgSO_4\cdot 7H_2O$	aph	Aphthitalite	$K_3Na(SO_4)_2$
arc	Arcanite	K_2SO_4	lso	--	Li_2SO_4
the	Thenardite	Na_2SO_4	mas	Mascagnite	$(NH_4)_2SO_4$
mir	Mirabilite	$Na_2SO_4\cdot 10H_2O$	cel	Celestite	$SrSO_4$
gla	Glauberite	$Na_2Ca(SO_4)_2$	bar	Barite	$BaSO_4$
syn	Syngenite	$K_2Ca(SO_4)_2\cdot H_2O$	bur	Burkeite	$Na_6CO_3(SO_4)_2$
pol	Polyhalite	$K_2Ca_2Mg(SO_4)_4\cdot 2H_2O$			
		Chlorides			
ant	Antarcticite	$CaCl_2\cdot 6H_2O$	sal	Salammoniac	NH_4Cl
bis	Bischofite	$MgCl_2\cdot 6H_2O$	sca	--	$SrCl_2\cdot 2H_2O$
tac	Tachyhydrite	$CaMg_2Cl_6\cdot 12H_2O$	sch	--	$SrCl_2\cdot 6H_2O$
syl	Sylvite	KCl	bca	--	$BaCl_2\cdot H_2O$
car	Carnallite	$KMGCl_3\cdot 6H_2O$	bch	--	$BaCl_2\cdot 2H_2O$
hal	Halite	$NaCl$	kai	Kainite	$KMgClSO_4\cdot 3H_2O$
lic	--	$LiCl_2\cdot H_2O$			
		Nitrates			
nic	Nitrocalcite	$Ca(NO_3)_2\cdot 4H_2O$	nil	--	$LiNO_3\cdot 3H_2O$
nim	Nitromagnesite	$Mg(NO_3)_2\cdot 6H_2O$	nia	Ammonia niter	NH_4NO_3
nit	Niter	KNO_3	nis	--	$Sr(NO_3)_2$
sod	Soda niter	$NaNO_3$	nib	Nitrobarite	$Ba(NO_3)_2$
		Borates			
iny	Inyoite	$Ca_2B_6O_{11}\cdot 13H_2O$[+]	bor	Borax	$Na_2B_4O_7\cdot 10H_2O$[+]
ind	Indirite	$Mg_2B_6O_{11}\cdot 15H_2O$[+]	ule	Ulexite	$NaCaB_5O_9\cdot 8H_2O$[+]
		Fluorides			
flu	Fluorite	CaF_2	vil	Villiaumite	NaF
sel	Sellaite	MgF_2	lif	--	LiF
		Phosphates			
hap	Hydroxyapatite	$Ca_5(PO_4)_3OH$[*]	fap	Fluorapatite	$Ca_5(PO_4)_3F$
mgp	--	$Mg_3(PO_4)_2$	wag	Wagnerite	Mg_2PO_4F
nap	--	Na_3PO_4			

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[*] Normative hydroxyapatite calculated as $Ca_{4.75}(PO_4)_{3.17}$.

[+] If calculated with average borate charge of -7/12 per boron; mineral compositions calculated as: inyoite, $Ca_{1.79}B_{6.14}O_{11}\cdot 13H_2O$; ulexite, $Ca_{0.98}Na_{0.98}B_{5.02}O_9\cdot 8H_2O$; indirite, $Mg_{1.79}B_{6.14}O_{11}\cdot 15H_2O$, and borax, $Na_{2.28}B_{3.91}O_7\cdot 10H_2O$.

combination with other solutes in the sample without interacting with the aqueous environment or requiring any chemical or charge modification. This latter criterion was adopted to exclude solutes that require interaction with water (hydrolysis, a pH effect; or H_2O dissociation, a redox effect), or a chemical and charge modification, because the character of the solute in the analysis differs form its character in the resultant solid phase. Thus, neither pH nor redox conditions enter directly into SNORM computations and cation-anion charge balance of the adjusted solute concentrations is preserved in the normative salt assemblage.

Fortunately, the solutes that were rejected from the normative calculation on the basis of the second criterion characteristically occur in no more than trace amounts. Uncommon exceptions are dissolved silica and alumina; iron, manganese, certain base metals, and transition elements; and reduced carbon and sulfur species. In waters where these constituents are present in significant amounts, the application of the normative calculation may be inappropriate.

Of the solutes that are distributed into normative salts (table 1) boron and the bicarbonate-carbonate pair, hereinafter referred to collectively as (bi)carbonate, are too widely distributed in natural waters to be excluded although they do not conform fully to the second criterion. Bicarbonate and carbonate are important constituents in most waters, and in most surficial or dilute waters and alkaline-saline lake waters they are the dominant anions. Boron, although not as abundant as (bi)carbonate, is a significant minor solute in many waters and reaches substantial concentrations in some continental evaporite waters. Assignment of (bi)carbonate to normative salts, however, requires additional manipulation of their concentrations to form the normative assemblage, and modification of normative borate salt compositions is sometimes required to maintain solute charge balance.

Carbonate-Bicarbonate Modifications

The concentrations of (bi)carbonate may require one or two modifications for assignment to normative salts. The first, if necessary, determines the fraction of carbonate in the total carbonate-bicarbonate concentration if total (bi)carbonate is expressed as bicarbonate. The second modification allows partitioning between carbonate and bicarbonate for assignmemt into the designated normative (bi)carbonate salts.

Carbonate fraction in total analyzed (bi)carbonate alkalinity

The first modification, is determined prior to adjusting solute concentrations to achieve cation-anion charge balance, and is made only if pH of the sample is recorded and total dissolved inorganic carbon (DIC) concentration is reported as bicarbonate, that is, no value for carbonate concentration is given. Under these circumstances the mole fraction of carbonate in the total analyzed DIC can be calculated. If, on the other hand, sample pH is not given, or carbonate concentration is reported, this calculation is omitted.

The carbonate-bicarbonate concentration ratio is calculated from the carbonate-bicarbonate equation,

$$HCO_{3\,(aq)}^{-} = CO_{3\,(aq)}^{2-} + H_{(aq)}^{+}$$

that defines the 25°C equilibrium

$$K_{eq} = \frac{(a_{CO_3^{2-}})(a_{H^+})}{(a_{HCO_3^-})} = 10^{-10.329} \qquad (1)$$

in which a is the individual ion activity for each of the designated solutes and K_{eq} is the equilibrium constant that has been assigned the value from Plummer and others (1976).

After activities are written in terms of molality, m_i,

$$a_i = \gamma_i m_i$$

with γ_i designating the individual ion activity coefficient of the ith ion, molalities are substituted for activities into equation (1), which is rearranged to

$$\frac{m_{CO_3^{2-}}}{m_{HCO_3^-}} = \frac{(\gamma_{HCO_3^-})K_{eq}}{(\gamma_{CO_3^{2-}})(a_{H^+})} \qquad (2)$$

and defines the carbonate-bicarbonate concentration ratio.

The term that remains to be evaluated before equation (2) can be solved is the ratio of ion activity coefficients, $\gamma_{HCO_3^-}/\gamma_{CO_3^{2-}}$. Each coefficient is calculated following procedures in WATEQ using the Debye-Hückel expression (Truesdell and Jones, 1974; Plummer and others, 1976). Use as a ratio of activity coefficients in equation (2) tends to cancel out systematic error in each of the individual values. The significance of error in these coefficients at high ionic strengths (alkaline-earth chloride-rich waters with very low (bi)carbonate concentrations) is further reduced and becomes negligible.

One source of error in solving equation (2) that may occasionally arise is if the analytical data are expressed in "per liter" units and water density is not reported. Molarity (moles per liter) is not equivalent to molality (moles per kilogram water), and the latter units cannot be directly calculated from the former without a density determination. Yet, definition of the ionic strength in the Debye-Hückel expression requires molalities. For such cases in which only molarities are known, we use a highly generalized empirical conversion,

$$m_i = M_i(1 + 0.022\Sigma eq_{cation})$$

in which m_i is the molality, M_i is the molarity, and Σeq_{cation} is the sum of the cation equivalents per liter in the analysis.

The result from equation (2), the carbonate-bicarbonate concentration ratio, is converted to the mole fraction of carbonate in the analyzed DIC. If the carbonate mole fraction exceeds 0.001, the fraction is used to calculate the carbonate and bicarbonate concentrations from the analytical bicarbonate value for use in further SNORM computations. Alternatively, if the carbonate mole fraction is less than 0.001, the entire calculation is abandoned, and the original analytical value of (bi)carbonate (DIC) is retained as bicarbonate concentration; the low carbonate mole fraction is considered insignificant and below the level of analytical error for the DIC determination.

Carbonate-bicarbonate assignment to normative salts

The reversible transition between adjusted carbonate and bicarbonate concentrations is required without effecting charge neutrality of the system. We have adopted the relationship

$$2HCO_3^-{}_{(aq)} = CO_3^{2-}{}_{(aq)} + H_2O_{(liq)} + CO_{2\,(gas)} \qquad (3)$$

that permits assignment of (bi)carbonate species into any (bi)carbonate salt(s) in the normative assemblage, yet conserves the total (bi)carbonate charge (only production or consumption of neutral carbon dioxide and water accompanies the transformation).

Boron Modifications

Boron assignment into normative salts presents a second problem. Boron is expressed as elemental boron in conventional water analyses but occurs as the borate radical in boron-bearing normative salts. Furthermore, each normative borate salt has one of three different boron-oxygen ratios in its respective borate radical with each exhibiting a different borate charge per boron (table 3). Thus, not only must boron in the analysis be recast as negatively charged borate to permit calculating a comprehensive cation-anion charge balance, but borate charge per boron for the recast solute is dependent on which borate salt(s) occur in the normative assemblage.

The stoichiometries of the four borate salts can be modified as shown in table 3, so that each contains a hypothetical borate radical of intermediate composition with a common charge per boron (-0.583). This permits recasting boron in the analysis to borate with the same charge per boron as in the modified borate salts. After adjusting solute concentrations to yield cation-anion charge balance, the boron can be assigned as borate to any of the modified borate salt stoichiometries. This produces a normative salt assemblage that adheres to the adjusted solute concentrations but contains borate salt(s) with slightly altered but balanced stoichiometry.

A norm that contains only a single borate salt (or the indirite-inyoite pair with identical borate stoichiometries) is recalculated with correct borate stoichiometry for the borate salt. Boron is again recast as a borate, but with the charge per boron mandated by the salt's correct stoichiometry. After readjusting solute concentrations to yield charge balance, the norm is recomputed with the normative borate salt reassigned to its correct stoichiometry. If, on the other hand, the norm does contain two or more borate salts (other than the indirite-inyoite pair), the initially computed norm is retained and the use of modified borate salt compositions (table 3) is specified in the output.

Cation-Anion Charge Balance

Charge neutrality among the solutes to be distributed into normative salts, already stressed as an important calculation in SNORM, is accomplished by summing the equivalency of cations (Σeq_{cation}) and anions (Σeq_{anion}) and determining their deviation from neutrality ($\Sigma eq_{cation}/\Sigma eq_{anion} = 1.0$). In this calculation boron is summed as the borate anion with an assigned borate charge per boron. Because the cause of deviation from cation-anion charge balance cannot be uniquely diagnosed, SNORM distributes the charge imbalance throughout all solutes. Those cation or anion concentrations with total excess charge are decreased proportionally, and the oppositely charged solute

Table 3. Normative borate salts, their chemical formula with anion charge per formula unit and per boron; and their modified chemical formula with anion charge per formula unit and per boron that yields identical borate charge per boron for each

Mineral	Formula	Borate charge per formula	Borate charge per boron	Modified formula	Modified borate charge per formula	Modified borate charge per boron
Indirite	$Mg_2B_6O_{11} \cdot 15H_2O$	-4	-0.667	$Mg_{1.79}B_{6.14}O_{11} \cdot 15H_2O$	-3.58	-0.583
Inyoite	$Ca_2B_6O_{11} \cdot 13H_2O$	-4	-0.667	$Ca_{1.79}B_{6.14}O_{11} \cdot 13H_2O$	-3.58	-0.583
Ulexite	$NaCaB_5O_9 \cdot 8H_2O$	-3	-0.600	$Na_{0.98}Ca_{0.98}B_{5.02}O_9 \cdot 10H_2O$	-2.94	-0.583
Borax	$Na_2B_4O_7 \cdot 10H_2O$	-2	-0.500	$Na_{2.28}B_{3.91}O_7 \cdot 10H_2O$	-2.28	-0.583

concentrations are correspondingly increased. Thus, the effect of the omission of one important solute from the analysis, or the faulty analysis of one solute, becomes distributed throughout all the solutes.

Normative Salts

SNORM assembles the salt norm for each water analysis from a list of 63 normative salts (table 2). The list contains the necessary array of salts to permit representation of the composition of any known natural water by an idealized equilibrium assemblage. The succeeding discussion reviews the features of the normative salt listing and the criteria that we adopted to formulate the list.

Occurrence as Salt Minerals

Whenever possible, the normative salts have been assigned compositions that occur naturally as minerals. However, several of the salts in table 2 do not occur naturally but only as normative salts because SNORM allows no interaction with host-rock salts, allows no consumption of solutes through authigenesis of clays and other silicates, allows no solid solution in the normative salts except for bromide and iodide in chlorides, and, unlike the natural process, "evaporates" the water to total dryness in a single step.

The largest group of these are the lithium salts; none occur as minerals. The lithium salts are moderately-to-highly soluble and, at the same time, lithium is never a dominant solute in natural waters. Its concentration rarely exceeds a few ppm except in a few playa evaporite waters associated with volcanics (Ericksen and others, 1976; Rettig and others, 1980), geothermal systems, and some deep basin "oil field" brines (Livingston, 1963; White and others, 1963) in which lithium concentrations reach several hundred ppm or more. Lithium substitutes readily for magnesium and ferrous iron in coexisting clay minerals and, to a lesser extent, in other minerals. Therefore, lithium never reaches a sufficiently high concentration for its salts to precipitate in natural systems--even from the saline evaporite brines that are noticeably enriched in lithium.

Similarly, the chloride and nitrate salts of barium and strontium, not known as minerals except for nitrobarite, are vastly more soluble than their respective sulfates and carbonates; thus, barium and strontium concentrations in natural waters characteristically remain low because of their direct precipitation as sulfates or carbonates, their substitution for calcium in carbonate (particularly strontium in aragonite) and sulfate minerals, and their replacement as carbonates and sulfates of preexisting carbonate and sulfate minerals in the host rock. Normative barium and strontium chlorides and nitrates occur in assemblages for concentrated waters drastically depleted in (bi)carbonate and sulfate, that is, waters containing normative calcium and magnesium chloride salts; they only occur in norms because no interaction with host rocks is permitted. In addition, the barium and strontium-bearing waters characteristically occur as deep basin (oil-field) brines that almost never reach the surface and undergo significant evaporative concentration and salt precipitation.

Sodium phosphate is included as a normative salt to accomodate those few waters in which phosphate remains after forming the normative calcium and magnesium phosphate salts. Magnesium phosphate, a salt that is unknown as a mineral, occurs in normative assemblages only if insufficient fluoride is present to form the magnesium fluorophosphate wagnerite.

Finally, the solutes bromide and iodide do not occur naturally as discrete bromide and iodide salts in sedimentary environments, but rather as solid solution components in chloride salts. We treat them similarly in SNORM; their adjusted concentrations are summed with that of chloride, and the total is assigned to the normative chloride salts in the assemblage.

Compound Salts

A wide variety of compound (double) salts are present in evaporite and other low-temperature environments; these salts range in abundance from the common dolomite, fluorapatite, and carnallite, to the rare tachyhydrite, kalistrontite, and pirssonite. The occurrence, genesis, and stability of many compound salts are well documented (see, for example, Braitsch, 1971; Eugster, 1980; Eugster and others, 1980; Harvie and others, 1984) and these must be included when forming the normative assemblage. Therefore, we have included all identifiably stable compound salt minerals that are composed solely of major solutes, that is--compound salts in the $Ca-Mg-K-Na-Cl-SO_4-HCO_3-CO_3-H_2O$ system, as well as several of the common compound-salt minerals, fluorapatite, wagnerite, and ulexite, that contain minor solutes. Of this latter group, wagnerite and the two apatites are SNORM's only normative calcium and magnesium phosphate minerals.

We have, however, excluded all compound salts that are not found as minerals, and most compound salt minerals that contain a minor solute, such as barytocalcite, $CaBa(CO_3)_2$, neighborite, $NaMgF_3$, and kalistrontite, $K_2Sr(SO_4)_2$, among others. This is done partially to reduce the number of phases in the listing of normative salts, but more importantly, to eliminate uncertainties about the stabilities and permissable mineral association of these rare minerals. Furthermore, standard chemical potentials of many compound salts are unknown. A principal reason for referring to the salt norm as an idealized equilibrium assemblage of salts is because these compound salts were omitted from the listing; some of these salts are undoubtedly stable at surface conditions.

Salt Stability Criteria

Each normative salt (table 2) is identified as the salt that is stable at 25°C and 1 bar pressure under the atmospheric partial pressure of carbon dioxide ($10^{-3.5}$ bars) within the water activity range of its occurrence in normative assemblages. The water activity, in turn, is determined by the composition of the terminal brine coexisting (saturated) with the full complement of salts in the normative assemblage and will be discussed more fully in the succeeding section. Most individual salt stabilities under the above constraints were determined from calculations using their standard chemical potentials at 25°C and 1 bar (10^5 pascals) as listed in table 4. These calculations only recently became possible for a large number of the salts, particularly the compound major-cation sulfate and chloride salts of marine and continental evaporite deposits, when standard chemical potentials became available through the work of Harvie and Weare (1980), and Harvie and others (1982, 1984).

The total array of calculations using table 4 to identify the stable salts that constitute table 2 need not be reviewed; the calculations identifying the normative sodium (bi)carbonate salt will illustrate our procedure and the data in table 4 will permit the reader to pursue other examples.

Five candidates exist among the sodium (bi)carbonate salts: nahcolite, $NaHCO_3$; trona, $Na_3H(CO_3)_2 \cdot 2H_2O$; natron, $Na_2CO_3 \cdot 10H_2O$; sodium carbonate heptahydrate, $Na_2CO_3 \cdot 7H_2O$; and thermonatrite, $Na_2CO_3 \cdot H_2O$. Using the chemical potentials in table 4, phase equilibria can be calculated and plotted (fig. 1) as water activity (a_{H_2O}) versus partial pressure of carbon dioxide (p_{CO_2}). Thermonatrite and the heptahydrate are only stable below atmospheric partial pressure of carbon dioxide ($10^{-3.5}$ bars, fig. 1) and are unacceptable as normative salts. Of the remaining three, natron is stable at water activities above 0.88 ($\log a_{H_2O} = -0.055$), nahcolite is stable at water activities below 0.15 ($\log a_{H_2O} = -0.815$), and trona is stable in the water activity interval between 0.15 and 0.88. Water activities as low as 0.15 in natural waters are approached only in saturated $CaCl_2$ brines (Harvie and others, 1984) in which no alkali (bi)carbonate salts are stable; therefore nahcolite as a normative salt is unacceptable. On the other hand, water activities are less than 0.8 in solutions saturated with sodium (bi)carbonate (Harvie and others, 1984), and natron is unstable. Only trona remains as the sodium (bi)carbonate salt in normative assemblages.

Table 4. Standard chemical potential values and sources

Volatile	Chemical formula	μ^o/RT	Source
Water (liquid)	H_2O	-95.6635	1
Carbon dioxide (gas)	CO_2	-159.092	1
Salt			
Ammonia niter	NH_4NO_3	-74.146	2
Anhydrite	$CaSO_4$	-533.73	1
Antarcticite	$CaCl_2 \cdot 6H_2O$	-893.65	1
Aphthitalite	$K_3Na(SO_4)_2$	-1057.05	1
Aragonite	$CaCO_3$	-455.17	1
Arcanite	K_2SO_4	-532.39	1
Barite	$BaSO_4$	-549.51	2
Barium chloride	$BaCl_2$	-326.94	3b
Barium chloride hydrate	$BaCl_2 \cdot H_2O$	-425.88	3b
Barium chloride dihydrate	$BaCl_2 \cdot 2H_2O$	-522.99	3b
Bischofite	$MgCl_2 \cdot 6H_2O$	-853.1	1
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	-1383.6	1
Borax	$Na_2B_4O_7 \cdot 10H_2O$	-590.95	3c
Burkeite	$Na_6CO_3(SO_4)_2$	-1499.4	1
Calcite	$CaCO_3$	-455.6	1
Calcium chloride tetrahydrate	$CaCl_2 \cdot 4H_2O$	-698.7	1
Carnallite	$KMgCl_3 \cdot 6H_2O$	-1020.3	1
Celestite	$SrSO_4$	-540.95	2
Dolomite	$CaMg(CO_3)_2$	-871.99	1
Epsomite	$MgSO_4 \cdot 7H_2O$	-1157.83	1
Fluorapatite	$Ca_5(PO_4)_3F$	-2604.3	2
Fluorite	CaF_2	-474.77	2
Gaylussite	$Na_2Ca(CO_3)_2 \cdot 5H_2O$	-1360.5	1
Glauberite	$Na_2Ca(SO_4)_2$	-1047.45	1
Gypsum	$CaSO_4 \cdot 2H_2O$	-725.56	1
Halite	$NaCl$	-154.99	1
Hexahydrite	$MgSO_4 \cdot 6H_2O$	-1061.60	1
Hydroxyapatite	$Ca_5(PO_4)_3OH$	-2535.8	2
Kainite	$KMgClSO_4 \cdot 3H_2O$	-938.2	1
Kalicinite	$KHCO_3$	-350.06	1
Kieserite	$MgSO_4 \cdot H_2O$	-579.8	1
Labile salt	$Na_4Ca(SO_4)_3 \cdot 2H_2O$	-1751.45	1
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	-1403.97	1
Lithium carbonate	Li_2CO_3	-456.7	3c
Lithium chloride	$LiCl$	-155.06	3c
Lithium chloride hydrate	$LiCl \cdot H_2O$	-254.88	3c
Lithium fluoride	LiF	-237.09	3c
Lithium nitrate	$LiNO_3$	-153.76	3c
Lithium nitrate trihydrate	$LiNO_3 \cdot 3H_2O$	-455.25	3c
Lithium sulfate	Li_2SO_4	-533.2	3c

Table 4 (continued).

Salt	Chemical formula	μ^o/RT	Source
Lithium sulfate hydrate	$Li_2SO_4\cdot H_2O$	-631.59	3c
Magnesite	$MgCO_3$	-414.45	1
Mascagnite	$(NH_4)_2SO_4$	-363.74	2
Mirabilite	$Na_2SO_4\cdot 10H_2O$	-1471.15	1
Nahcolite	$NaHCO_3$	-343.33	1
Natron	$Na_2CO_3\cdot 10H_2O$	-1382.78	1
Nesquehonite	$MgCO_3\cdot 3H_2O$	-695.3	1
Niter	KNO_3	-159.16	2
Nitrobarite	$Ba(NO_3)_2$	-321.34	2
Nitrocalcite	$Ca(NO_3)_2\cdot 4H_2O$	-691.22	3b
Nitromagnesite	$Mg(NO_3)_2\cdot 6H_2O$	-839.36	3b
Picromerite	$K_2Mg(SO_4)_2\cdot 6H_2O$	-1596.1	1
Pirssonite	$Na_2Ca(CO_3)_2\cdot 2H_2O$	-1073.1	1
Polyhalite	$K_2Ca_2Mg(SO_4)_4\cdot 2H_2O$	-2282.5	1
Potassium carbonate hydrate	$K_2CO_3\cdot 3/2H_2O$	-577.37	1
Potassium sesquicarbonate	$K_8H_4(CO_3)_6\cdot 3H_2O$	-2555.4	1
Potassium sodium carbonate	$KNaCO_3\cdot 6H_2O$	-1006.8	1
Potassium trona	$K_2NaH(CO_3)_2\cdot 2H_2O$	-971.74	1
Salammoniac	NH_4Cl	-82.201	2
Sellaite	MgF_2	-432.07	2
Soda niter	$NaNO_3$	-148.11	2
Sodium carbonate heptahydrate	$Na_2CO_3\cdot 7H_2O$	-1094.95	1
Sodium phosphate	Na_3PO_4	-721.64	3c
Strontionite	$SrCO_3$	-458.93	2
Strontium chloride	$SrCl_2$	-315.12	3b
Strontium chloride dihydrate	$SrCl_2\cdot 2H_2O$	-517.15	3b
Strontium chloride hexahydrate	$SrCl_2\cdot 6H_2O$	-904.13	3b
Strontium nitrate	$Sr(NO_3)_2$	-314.29	3b
Sylvite	KCl	-164.84	1
Syngenite	$K_2Ca(SO_4)_2\cdot H_2O$	-1164.8	1
Tachyhydrite	$CaMg_2Cl_6\cdot 12H_2O$	-2015.9	1
Teschemacherite	NH_4HCO_3	-268.7	3a
Thenardite	Na_2SO_4	-512.35	1
Thermonatrite	$Na_2CO_3\cdot H_2O$	-512.8	1
Trona	$Na_3H(CO_3)_2\cdot 2H_2O$	-960.38	1
Villiaumite	NaF	-220.39	2
Witherite	$BaCO_3$	-456.74	2

Sources - 1. Harvie and others (1984).
2. Robie and others (1978).
3. NBS Technical Note 270: a. Wagman and others (1968); b. Parker and others (1971); c. Wagman and others (1981).

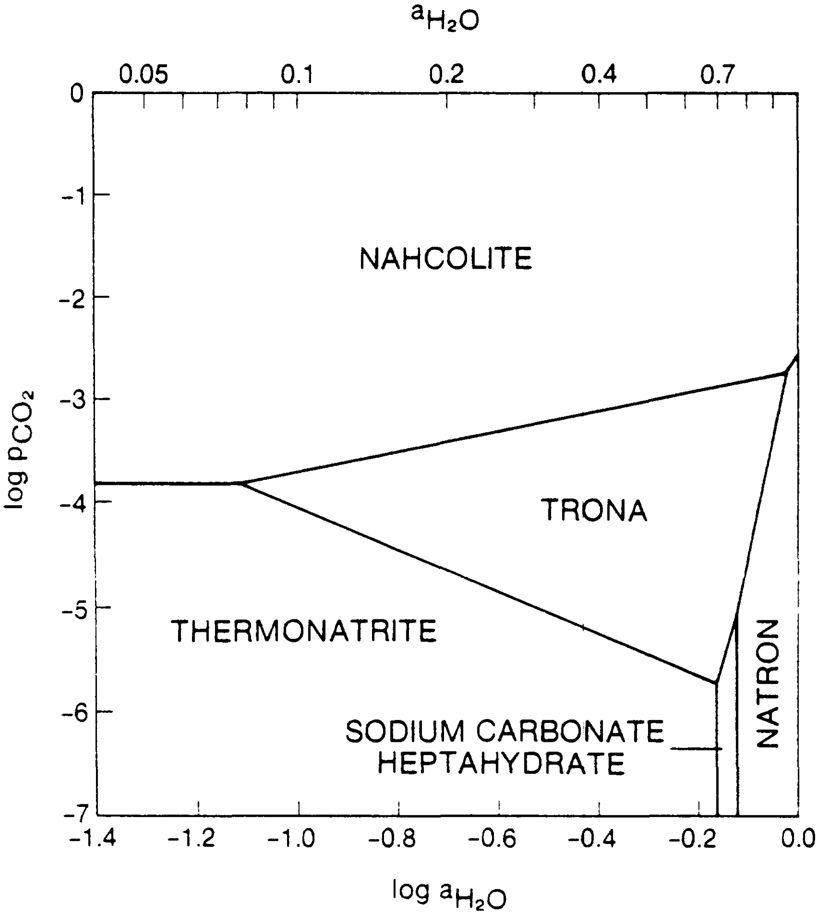

Figure 1. Calculated stability relations among the Na_2CO_3-$NaHCO_3$-H_2O salts at 25°C and 1 bar pressure as functions of water activity and fugacity of carbon dioxide in the coexisting aqueous phase.

Examples of results using parallel, but generally less complex calculations include: designation of kalicinite as the normative salt, rather than a variety of potassium (bi)carbonate salts; elimination of any sodium-potassium (bi)carbonate salts as normative salts; designation of pirssonite as the normative salt rather than gaylussite; and designation of kieserite and epsomite, leonite and picromerite, gypsum and anhydrite, thenardite and mirabilite, and the appropriate hydrates of $BaCl_2$, $SrCl_2$, LiCl, Li_2SO_4, and $LiNO_3$ in table 2 as permissable alternative hydrates. The designation of the normative $MgSO_4$ hydrates, epsomite and kieserite, produced an unusual result. Hexahydrite, a not uncommon evaporite mineral with a hydration level between that of kieserite and epsomite (table 4), precipitates during progressive evaporation of seawater at 25°C (Braitsch, 1971; Harvie and others, 1982) but within an interval that is between the water activities in brines coexisting with alkaline-earth bearing chlorides and alkali-bearing sulfates.

In some instances aqueous ion activities also had to be considered along with the crystalline salts, water activity, and, in reactions involving (bi)carbonate salts, the partial pressure of carbon dioxide, to designate the normative salt. Hydroxyapatite, rather than whitlockite, $Ca_3(PO_4)_2$, as the stable calcium phosphate is an example. Hydroxyapatite is a common sedimentary mineral and whitlockite is relatively rare; the latter's occurrence as a sedimentary mineral appears to be restricted to modern insular guano deposits (Gulbrandsen, 1975). The equilibrium between hydroxyapatite and whitlockite,

$$\underset{\text{hydroxyapatite}}{2Ca_5(PO_4)_3OH} + 2H^+ = \underset{\text{whitlockite}}{3Ca_3(PO_4)_2} + Ca^{2+} + 2H_2O$$

is plotted in terms of pH and the logarithm of the aqueous calcium ion activity to define hydroxyapatite and whitlockite stability fields for two extremes of water activity, $a_{H_2O} = 1.0$ and 0.1 (fig. 2). Calcite saturation at atmospheric partial pressure of carbon dioxide at the same two water activities is also shown; calcite saturation lies well within the hydroxyapatite field at more than two orders of magnitude greater calcium ion activity than the hydroxyapatite-whitlockite equilibrium. Thus, with any calcium-bearing salt in the normative assemblage, hydroxyapatite, rather than whitlockite is the stable calcium phosphate salt. All Ca-bearing salts are nearly as soluble or more soluble than calcite except fluorite, and if fluorite occurs in the assemblage, fluorapatite, not hydroxyapatite, is the stable phosphate. These results parallel Gulbandsen's observation that whitlockite appears to be a metastable intermediate in the transition from guano to apatite.

In those cases in which standard chemical potentials of one or more related salts were not available, evidence from geologic observations and experimental results was used. The unusual evaporite minerals chlorocalcite ($KCaCl_3 \cdot 6H_2O$) and georgeyite ($K_2Ca_5[SO_4]_6 \cdot H_2O$), for example, were not designated as normative salts because their occurrence appears to be restricted to thermally metamorphosed salts (Braitsch, 1971). Bloedite was selected as the normative Na-Mg sulfate, rather than vanthoffite or loewite, and leonite and picromerite as the normative K-Mg sulfates, rather than langbeinite, based on experimental data and nature of their occurrence reported by Braitsch (1971).

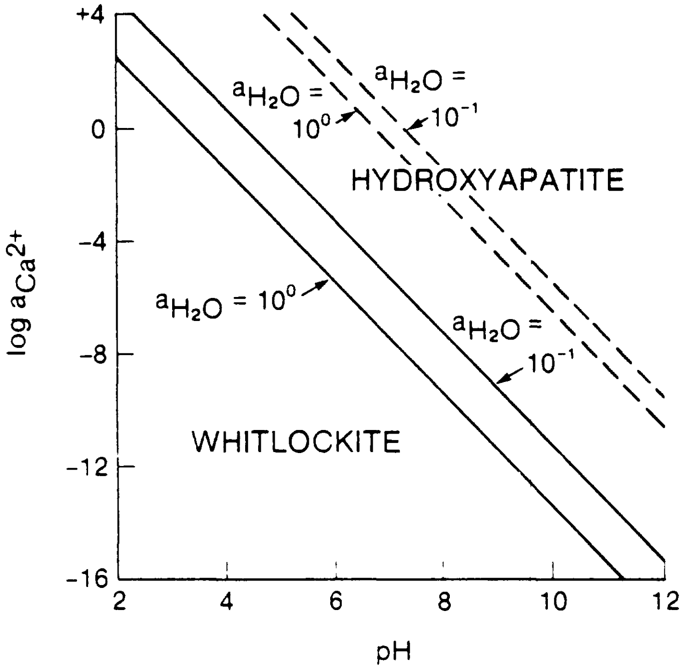

Figure 2. Hydroxyapatite-whitlockite stability relations (solid lines) at 25°C and 1 bar pressure as a function of the logarithm of calcium ion activity and pH in the coexisting aqueous fluid at two extreme water activities (10^0 and 10^{-1}); calcite saturation (dashed lines) at atmospheric partial presure of carbon dioxide ($10^{-3.5}$ bars) plotted for the same two water activity extremes.

Designation of the normative borate salts cannot be rigorously resolved. Not only have a vast number of borate minerals, some with complex compositions, been identified from evaporite deposits (see, for example, Sonnenfeld, 1984, p. 470-471), but nearly all are lacking standard free energy values. Therefore, we have designated only four normative borates (table 2) that, from observations of natural occurrences, are representative of, rather than rigorously defined by the normative assemblage.

We have arbitrarily limited the normative borate salts to the quinary system, $CaO-MgO-Na_2O-B_2O_3-H_2O$. This excludes all double anion borates such as boracite, lueneburgite, heidenite, and the array of borosilicates; the rarely occurring potassium-bearing borates, kaliborate and santite; and all minor cation borates such as the various strontium-bearing borates infrequently encountered in the Zechstein salts (Braitsch, 1971). Except for ulexite, we have also excluded all double cation borates; ulexite has been included because of its frequent abundance in many playa and spring deposits (Muessig, 1959; Bowser and Dickson, 1966).

For each endmember borate composition we have designated its most abundant and frequently occurring anhydrous stoichiometry as the normative salt composition. The anhydrous stoichiometery $2CaO \cdot 3B_2O_3$ (the minerals inyoite, mayerhoffite, and colemanite) is far more abundant than other calcium borate stoichiometries. Although the magnesium borates ascherite and boracite are the most abundant borate minerals in marine evaporite rocks, there is convincing evidence that these minerals are secondary having formed in response to thermal metamorphism and postdepositional fluid transport and deposition (Kühn, 1968; Braitsch, 1971; Sonnenfeld, 1984). In recent playa and spring deposits, on the other hand, the anhydrous stoichiometry $2MgO \cdot 3B_2O_3$ (the minerals indirite and kurnakovite) is the most frequently occurring composition of the relatively rare magnesium borates (Muessig, 1959, 1966). The $Na_2O \cdot 2B_2O_3$ anhydrous stoichiometry (the minerals borax, tincalconite, and kernite) is unquestionably the most abundant of the sodium borate compositions in recent playa and spring deposits and is the major commercial source of boron (Muessig, 1959; Smith and Haines, 1964; Bowser and Dickson, 1966). These three anhydrous stoichiometries plus $Na_2O \cdot 2CaO \cdot 5B_2O_3$ (the minerals ulexite and probertite) constitute the anhydrous stoichiometries of the normative borate salts.

Designation of the "stable" hydrate for each of the four borate stoichiometries is based on observations by Muessig (1959). He concluded that, based on sedimentological, textural, and other paragenetic criteria at playa evaporite deposits along with some experimental data, the most hydrated in each of the colemanite, indirite, borax and ulexite hydration series is the primary borate salt; lesser hydration states are presumably secondary. We are not convinced his conclusions are valid throughout the range of water activities associated with normative salt assemblages. For example, the low water activity associated with normative Mg-Ca chloride salt assemblages is far below that observed at playa occurrences and may well be in equilibrium with borate salts of lower hydration. Nevertheless, until more definitive data for the borate mineral stabilities become available, we have incorporated Muessig's conclusions into SNORM by designating inyoite, indirite, borax, and ulexite (table 2) as the normative hydration states of the four anhydrous stoichiometries.

Salt Composition Modifications

Hydroxyapatite (table 2) is the only normative salt, other than the borates, whose composition cannot be constructed solely from a combination of solutes; hydroxyapatite contains one hydroxide radical per formula unit. In order to preserve cation-anion charge balance in the system, hydroxyapatite's composition is modified to $Ca_{4.75}(PO_4)_{3.17}$ (the whitlockite composition) from $Ca_5(PO_4)_3(OH)$. This change is not large and apatite's abundance in salt norms is characteristically minor; thus, the modification has little effect. Furthermore, fluorapatite, which does retain its correct stoichiometry in normative assemblages, is the stable apatite in any sample which contains sufficient fluoride, and results in only infrequent occurrence of normative hydroxyapatite.

Normative Salt Assemblages

The salt norm for each sample consists of the equilibrium assemblage of normative salts from table 2, the abundances of which are quantitatively equivalent to the adjusted solute abundances (concentrations). Assignment of the correct salts to the norm occurs in three steps: (1) The group of salts from table 2 that are eligible candidates based on solute species in the analysis and gross solute concentration relationships is defined; (2) the Gibbs phase rule is applied to determine the number of salts that comprise the assemblage; and (3) the single assemblage of elgible salts that contains only permissable salt associations and is quantitatively equivalent to solute concentrations is identified.

Eligible Salts

Salts from table 2 are selected to form a group of eligible candidates for possible assignment to the salt norm for each analysis. In this manner a substantial number of the 63 salts in table 2 are eliminated from further consideration. Because equilibrium hydration levels are assigned later, only the less hydrated salt from each of seven pairs of salts with two potentially permissable hydration states is retained in the list of eligible salts; anhydrite, for example, is retained as an eligible salt but gypsum is deleted. Two criteria are then applied to each analysis to further reduce the number of eligible salts.

The first criterion is that each eligible salt must be composed exclusively of components that occur as solutes in the analysis. This eliminates any salt that is composed of one or more solutes that are not represented in the analysis.

The second criterion is that each eligible salt is compatible with selected solute equivalency relations in each of four sets of solutes. Each relation compares a sum of solute equivalencies between a designated group of cations and a designated group of anions (table 5), and, if the specified relation is fulfilled, the group of salts identified with the relation are

Table 5. Salts excluded from assemblages in SNORM as a function of charge ratios of selected cation and anion groups of solutes

I. $\Sigma eq_{(Ca + Mg + Ba + Sr + Li)} > \Sigma eq_{(PO_4 + SO_4 + CO_3 + F + B^*)}$

Trona
Pirssonite
Kalicinite
Witherite
Teschemacherite
Thenardite
Arcanite
Glauberite
Syngenite
Bloedite
Leonite
Aphthitalite
Mascagnite
Burkeite
Ammonia niter
Ulexite
Borax
Villiaumite
LiF
Na_3PO_4

II. $\Sigma eq_{(Ca + Mg + Ba + Sr + Li)} < \Sigma eq_{(PO_4 + SO_4 + CO_3 + F + B^*)}$

Antarcticite
Tachyhydrite
Bischofite
$SrCl_2 \cdot 2H_2O$
$BaCl_2 \cdot H_2O$
Nitrocalcite
Nitromagnesite
$Sr(NO_3)_2$
Nitrobarite

III. $\Sigma eq_{(Ca + Mg + Sr)} < \Sigma eq_{(PO_4 + CO_3)}$

Anhydrite
Kieserite
Glauberite
Syngenite
Polyhalite
Bloedite
Leonite
Celestite
Carnallite
Kainite
Inyoite
Ulexite
Indirite
Fluorite
Sellaite

IV. $\Sigma eq_{(Ca + Mg)} > \Sigma eq_{(PO_4 + CO_3 + F)}$

Trona
Pirssonite
Kalicinite
Strontionite
Witherite
Teschemacherite
Li_2CO_3
Brukeite
Villiaumite
LiF
Na_3PO_4

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*Borate assigned an average charge of -7/12 per boron (see text).

deleted from the list of eligible candidates for that particular norm. These relations follow the major compositional "divides" that were defined by Hardie and Eugster (1970), and Eugster and Hardie (1978).

The first relation (I in table 5) defines an alkaline-earth chloride water in which the alkali-bearing (bi)carbonate and sulfate salts, among others, are unstable and not considered. The second relation (II) is the inverse of (I) and defines a water in which the alkaline-earth chloride salts are not considered. The third and fourth relations define the two major varients of II; either an alkali (bi)carbonate water (III) in which the alkaline-earth bearing sulfate salts, among others, are not considered, or an alkali sulfate water in which the alkali-bearing (bi)carbonate and other salts are not considered.

The procedures by which the four groups of ineligible salts were identified rely chiefly on the free energies of reaction at standard conditions calculated with standard chemical potentials (table 4). As an example, consider the two equilibria

$$\underset{\text{glauberite}}{Na_2Ca(SO_4)_2} + \underset{\text{antarcticite}}{CaCL_2 \cdot 6H_2O} = \underset{\text{anhydrite}}{2CaSO_4} + \underset{\text{halite}}{2NaCl} + 6H_2O$$

and

$$\underset{\text{bloedite}}{Na_2Mg(SO_4)_2 \cdot 4H_2O} + \underset{\text{bischofite}}{MgCl_2 \cdot 6H_2O} = \underset{\text{kieserite}}{2MgSO_4 \cdot H_2O} + \underset{\text{halite}}{2NaCl} + 8H_2O$$

that yield free energies of reaction of -25.6 and 4.5 kilojoules respectively. These values are substituted into the equality defining the natural log of the equilibrium constant, ln K_{eq}, in terms of the free energy of reaction at standard conditions, ΔG_r^o,

$$\ln K_{eq} = -RT\Delta G_r^o$$

with R, the gas constant, and T, the temperature in degrees Kelvin. The equilibrium constant, in turn, defines the activity of water in both equilibria, $K_{eq} = (a_{H_2O})^6$ and $(a_{H_2O})^8$, respectively. Water activities are 5.6 and 0.8 respectively for the two reactions at equilibrium. The high water activities (a maximum water activity at bischofite saturation is 0.34) at equilibrium preclude stablility of the glauberite-antarcticite and bloedite-bischofite pairs, and contribute to the documentation that alkali-bearing sulfates are unstable in alkaline-earth chloride waters (I in table 5), and conversely, that alkaline-earth chlorides are unstable in alkali-bearing sulfate waters (II). Whenever possible, parallel equilibria were calculated to identify the ineligible salts for each of the four relations.

For those salts without standard chemical potential data, ineligiblities were arbitrarily assigned based on relations in other groups. For example, borax and ulexite were ruled ineligible in alkaline-earth chloride waters, and inyoite, ulexite, and indirite were ruled ineligible in alkali carbonate waters.

Number of Salts in the Assemblage

The number of salts in each normative assemblage is calculated through use of the Gibbs phase rule

$$P = C - F + 2$$

in which P is the maximum number of phases in the assemblage, C is the minimum number of components whose abundances are independent variables and collectively define the phases quantitatively, and F is the number of degrees of freedom that can be independently imposed on the system.

Two degrees of freedom, temperature and pressure, are identified for the salt norm system. These are arbitrarily assigned (25°C and 1 bar) as independent variables and are not fixed by the character of the normative assemblage.

The number of components in the salt norm system, in addition to water, may be initially envisioned as the number of solutes in the analysis. However, because of the character of the normative assemblage and some previously adopted conventions, the number of components in the phase rule calculation comply with the following stipulations.

Because the sum of adjusted concentrations of chloride, bromide, and iodide are distributed into the chloride salts as mutually indistinguishable solutes, their collective abundance represents a single component rather than three individual solute components. Similarly, because the adjusted concentrations of carbonate and bicarbonate can be mutually exchanged one with the other through equation (3) to conform to the stoichiometry of the designated (bi)carbonate salts, the collective abundance of carbonate and bicarbonate defines a single component. The number of remaining single ion solute components is then lowered by one for use in the phase rule because some one arbitrarily designated solute concentration can be considered as a dependent variable that establishes cation-anion charge balance. Finally, water is not considered a component in the phase rule calculation; because no free water coexists with the normative assemblage, water's abundance is a dependent variable that is defined solely by the number of hydration waters required to form the normative salts.

Prohibited Salt Associations

After determining which salts are eligible in an assemblage of a given initial composition (table 5) and the number of salts that constitutes the assemblage, only one assemblage can be formed that is qualitatively and quantitatively compatible with the adjusted solute concentrations, and that excludes all prohibited salt associations throughout the assemblage.

The criterion that the assemblage excludes all prohibited (unstable) salt associations in the assemblage is fulfilled if the assemblage contains none of the prohibited associations shown in table 6. The table is a compendium of all salt associations that are prohibited, or assumed prohibited at $25^{o}C$ and 1 bar pressure. Most of the unstable associations are salt pairs that are identified in the matrix of normative salts; a few are prohibited three-salt and four-salt associations that are listed outside the matrix. Alternative hydration states for those salts with more than one stable hydration state are not specified in table 6; designation of hydration states for these salts will be discussed subsequently.

Calculations producing table 6 follow the same general procedures discussed previously for the development of table 5. Whenever possible, the unstable associations in table 6 were calculated by determining the equilibrium with the standard chemical potential data from table 4; an unstable association has higher free energy in the appropriate chemical environment (water activity, carbon dioxide partial pressure) than its stable isochemical equivalent. For salts lacking standard chemical potential data, in particular, the borates and phosphates, unstable associations were identified by analogy with prohibited associations in other groups and relationships observed in low-temperature natural assemblages. Major features of the phase relations among the normative salts that result from these calculations or assumptions are given in Appendix V.

The compositional constraints for the assemblage require that all solutes are qualitatively represented in the collective composition of salts in the assemblage, and that salt abundances can be quantitatively calculated from the solute abundances. Only a single assemblage that contains no prohibited associations from table 6 will satisfy this latter constraint, and this assemblage, after assigning proper hydration levels to salts with more than one hydration state, becomes the normative assemblage.

Hydration-Dehydation Equilibria

The final step in defining the salt norm is assignment of the equilibrium hydrate for any of the six salt compositions that can occur in one of two possible hydration states (table 7). Each hydration-dehydration transformation in table 7 is defined by its equilibrium water activity; thus, the water activity in the most concentrated brine that coexists with and is saturated with the full normative assemblage determines the stable hydration level of each salt pair. However, SNORM neither considers brine evolution nor calculates the composition and thermochemical properties of the terminal brine; SNORM only considers initial water composition and distributes the solutes into the equilibrium salt assemblage. The stable hydration state for these salts must be assigned using criteria from the normative assemblage itself, rather than from unknown thermochemical and compositional properties of an undefined terminal brine.

Table 7. Water activities (a_{H_2O}) and indicator salts* for hydration-dehydration equilibria in SNORM

	Equilibrium	a_{H_2O}#	Indicator salts*
1.	$BaCl_2 \cdot H_2O + H_2O = BaCl_2 \cdot 2H_2O$	0.23	Antarcticite, tachyhydrite
2.	$SrCl_2 \cdot 2H_2O + 4H_2O = SrCl_2 \cdot 6H_2O$	0.34	Nitrocalcite, $BaCl_2 \cdot 2H_2O$
3.	$MgSO_4 \cdot H_2O + 6H_2O = MgSO_4 \cdot 7H_2O$ kieserite epsomite	0.57+	Bischofite, carnallite, nitromagnesite
4.	$K_2Mg(SO_4)_2 \cdot 4H_2O + 2H_2O = K_2Mg(SO_4)_2 \cdot 6H_2O$ leonite picromerite	0.67	Epsomite-any chloride salt, kainite
5.	$CaSO_4 + 2H_2O = CaSO_4 \cdot 2H_2O$ anhydrite gypsum	0.78	Any chloride or nitrate salt
6.	$Na_2SO_4 + 10H_2O = Na_2SO_4 \cdot 10H_2O$ thenardite mirabilite	0.81	Any alkali-bearing (bi)carbonate salt

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*Occurrence of any indicator salt in the assemblage denotes stability of the less hydrous hydrate for the designated equilibrium and for all other hydration-dehydration equilibria at higher water activities.

#Calculated from equilibrium relation with chemical potential data in table 4.

+Hexahydrite is stable in the water activity interval 0.50-0.57; however, no reasonable salt assemblage appears to generate a terminal, invarient brine within this water activity interval.

Water activity in a brine varies markedly as a function of brine composition, and a brine′s invarient terminal composition, therefore its water activity, are fixed by the assemblage of coexisting salts. For example, a terminal brine coexisting with the antarcticite-tachyhydrite pair has a water activity <0.2; on the other hand, a terminal brine coexisting with a variety of sulfate salts and no chloride or nitrate salts in the assemblage has a water activity >0.8 (Harvie and others, 1982).

Thus, the array of salts constituting the assemblage defines the water activity in the terminal brine, and the presence or absence of selected "indicator" salts in the assemblage allows confident assignment of the stable hydration level to each of the six pairs of salts in table 7. The presence of any indicator salt in the assemblage dictates stability of the lower hydration state for that hydration-dehydration pair and for each succeeding pair at higher equilibrium water activities in table 7; conversely, the absence of any indicator salt for that equilibrium and for any preceeding hydration-dehydration equilibrium at lower water activity dictates the stability of the higher hydration state in the normative assemblage.

Simple Salt Assemblages

The simple salt assemblage that is calculated by SNORM is recast from the normative salt assemblage and offers an abbreviated, simplified representation of the salt norm that may be useful in comparing waters or tracing their evolution. The simple salt assemblage is a quantitative listing of the constituent anhydrous simple salt components in those normative salts that are composed exclusively of major solutes. For example, a mole of normative polyhalite yields two moles of $CaSO_4$ and one mole of each $MgSO_4$ and K_2SO_4 that are assigned to the simple salt assemblage; a mole of normative borax, on the other hand, is ignored. Each simple salt is defined with an anion charge of -2 to maintain consistency throughout an array of simple salts; this results in molar units of the alkali chlorides being expressed as Na_2Cl_2 and K_2Cl_2. Twelve different simple salts are recognized: the carbonates (normative bicarbonate is expressed as carbonate in the simple salts), sulfates, and chlorides (chloride includes any bromide and iodide in solid solution) of each of calcium, magnesium, potassium, and sodium.

The advantages of the simple salt assemblage are twofold. First it offers a managable basis (12 different simple salts *vs* 63 different normative salts) for characterizing waters graphically for comparative and descriptive purposes, as well as a shorthand for describing a water--a Na_2CO_3 water or a $CaCl_2$ water. Second, it offers to those lacking a mineralogic background a useful and understandable alternative to the compositional complexities and nomenclature of saline minerals.

sulfate or carbonate, a spread in solute concentration of three orders of magnitude. Perhaps, the most profound consequence of this exercise will be the prediction of further evolution of solute composition out of contact with initial precipitates, particularly those containing more sparingly soluble constituents. However, interpretation becomes questionable for very dilute waters in which solute sources are dominated by aerosol dissolution, biologic degradation, or anthropogenic contaminants. Some effects of such initial contributions may remain despite extensive subsequent reaction in the normal weathering environment.

Hardie and Eugster (1970) have underscored the importance of the calcite and gypsum solubility "divides" in the subsequent solute evolution of concentrating waters. The required removal of Ca and carbonate or sulfate in equal proportions at the time of precipitation assures the continued dominance of whichever of the two constituents is most abundant at that point. As Ca must exceed both CO_3 and SO_4 to prevail at both junctures, it is easy to understand why calcium-dominated saline solutions are relatively uncommon. In fact, the excess of equivalent sulfate over calcium in seawater leads to its clear alkali-magnesium sulfo-chloride character with evaporative concentration. The importance of the two common, relatively insoluble calcium salts to the compositional evolution of natural waters is illustrated by a trilinear diagram (fig. 3) taken from R. J. Spencer (Univ. of Calgary, personal commun. 1982). The plot of water compositions on this diagram will qualitatively predict the major-solute matrix of all saline waters. The calculation of salt norms permits these predictions to be made in a more quantitative way.

Readily discernible differences of genetic importance can be illustrated in the comparison of salt norms (table 8) for seawater and for the average world river compositions given by Livingstone (1963). The abundance of alkaline-earth carbonates, as represented by calcite and dolomite, the presence of alkali-bearing double sulfates glauberite and syngenite, and the relatively minor amount of halite as the sole chloride in the river-water norm differ markedly from the chloride-rich, carbonate-poor seawater assemblage. The contrast illustrates the fundamental difference in ultimate anionic source for reacting solutions (H_2CO_3 vs. HCl), and the more geochemically evolved state of the oceans as compared to most continental waters (Mackenzie and Garrels, 1966). It generally is agreed that the oceans achieved their present chloride concentration very early in earth history by degassing at HCl/H_2O ratios very close to present crustal values (Holland, 1984). Subsequent additions of primordal chloride to the hydrosphere compared to the mass of Cl in the oceans or sedimentary rocks can be considered negligible.

At the same time there are two distinct disadvantages to exclusive use of the simple salt assemblage. First, any major solutes that are combined with minor solutes, such as sodium in normative borax or soda niter, are omitted from the simple salt assemblage. Second, the simple salt assemblage cannot be viewed as an equilibrium assemblage; recasting any normative compound salt into its simple salts immediately precludes an equilibrium association among the simple salts. Furthermore, the simple salt assemblage may well be an infraction of the Gibbs phase rule; the number of simple salts in the assemblage frequently exceeds the phase rule maximum. The simple salt assemblage should be considered as a useful supplement to, rather than a substitute for the salt norm.

INTERPRETATION OF SALT NORMS

Attempts to interpret the origin of the principal constituents dissolved in natural waters frequently have used ion ratios and graphical techniques. These considerations commonly rely on diagnostic relations between individual solutes, which remain relatively unaffected or follow known trends through subsequent geochemical evolution of the water mass. Such trends and relationships accompanying the extensive concentration of natural surface and subsurface waters have been generalized by Hardie and Eugster (1970), Eugster and Hardie (1978), Carpenter (1978), Eugster and Jones (1979), and Al Droubi and others (1980). These papers emphasize the control of major-element distribution in waters by precipitate mineral mass balances (particularly calcite, gypsum, and halite), and the potential of using constituents conserved in solution for tracing the geochemical history of any water.

The law of mass action requires that cations and anions be added or subtracted from solution in stoichiometric proportion by the congruent dissolution or precipitation of a mineral. Thus, molar proportions of ions in a given water reflect the composition of original simple salt minerals or the products of nonsalt mineral dissolution by natural acid (carbonic from the hydrolysis of CO_2 or sulfuric from oxidation and hydrolysis of sulfides). The computational association of cations and anions into a salt norm, such as is done in SNORM, quantitatively projects an eventual disposition of the dissolved constituents according to the most stable salt assemblage at $25^{\circ}C$ and one bar pressure.

Outside a system closed to all components except H_2O, the computation does not directly address the geochemical evolution of a natural water, but much may be inferred from some knowledge of relative solubility sequence, precipitation kinetics, and geologic setting. Such interpretation must allow for the differences in environmental influences likely to accompany the range in solubility between alkaline-earth carbonate, calcium sulfate, and alkali

Table 8. Major solute concentrations and major-ion normative salts for mean compositions of seawater and world river waters

[Seawater from Riley and Chester, 1971; river waters from Livingstone, 1963]

			River waters*				
Solutes (mg/kg)		Seawater	North America	South America	Europe	Australia	WORLD
	Mg	1,293.	5.	1.5	5.6	2.7	4.1
	Ca	411.	21.	7.2	31.1	3.9	15.
	Na	10,760.	9.	4.	5.4	2.9	6.3
	K	399.	1.4	2.	1.7	1.4	2.3
	Cl	19,350.	8.	4.9	6.9	10.	7.8
	HCO_3	143.	68.	31.	95.	31.6	58.4
	SO_4	2,709.	20.	4.8	24.	2.6	11.2
	TDS#	35,150.	133.4	56.1	173.4	55.2	106.1
Normative salts, anhydrous (wt. %)							
Calcite	$CaCO_3$	-	17.7	29.5	25.0	-	18.2
Dolomite	$CaMg(CO_3)_2$	-	36.9	29.4	34.2	48.6	40.8
Magnesite	$MgCO_3$	0.3	-	-	-	4.9	-
Anhydrite	$CaSO_4$	4.0	6.8	-	24.2	8.3	3.2
Kieserite	$MgSO_4$	6.1	-	-	-	-	-
Syngenite	$K_2Ca(SO_4)_2$	-	2.8	-	-	-	8.7
Glauberite	$Na_2Ca(SO_4)_2$	-	20.5	2.9	2.9	-	10.1
Aphthitalite	$K_3Na(SO_4)_2$	-	-	11.6	-	-	-
Thenardite	Na_2SO_4	-	-	4.3	-	-	-
Bischofite	$MgCl_2$	6.5	-	-	-	-	-
Carnallite	$KMgCl_3$	4.9	-	-	-	8.4	-
Sylvite	KCl	-	-	-	-	5.1	-
Halite	NaCl	78.1	13.6	19.5	9.1	24.6	16.8
	Sum#	99.9	98.3	97.2	95.4	99.9	97.8

*Africa and Asia not listed because potassium not given (Africa) or combined with sodium (Asia).

#TDS includes minor solutes; salt norms total <100% because minor-solute normative salts not listed (chiefly indirite and celestite in seawater, and niter and soda niter in river waters).

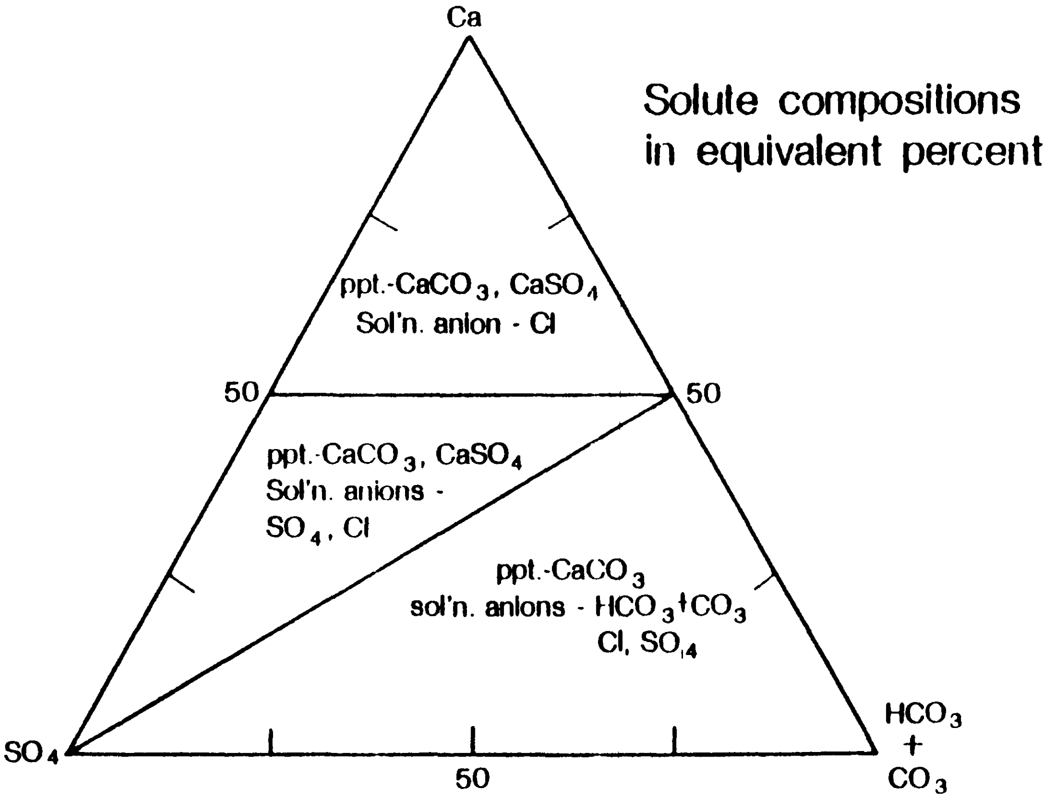

Figure 3. Trilinear diagram from R. J. Spencer differentiating the solute compositions of natural waters according to the relative proportions of calcium, carbonate species, and sulfate. The diagram illustrates the importance of the calcite and gypsum "divides" to evolving solution composition. The fields of the diagram are labeled with precipitates and dominant solution anions to be expected on further evaporation.

The extent of variance in salt norms for continental waters in table 8 can be seen through the differences in assemblage, as well as amounts, for the average river waters of some continents. Note the more sodic North American waters (led by the Mississippi River system) are characterized by abundant glauberite, the more potassic waters from South American (dominated by the Amazon) produce aphthitalite, and the more chloridic Australian waters (principally the River Murray) make normative sylvite. Despite a variance of 3 times in carbonate-species concentration, the four average river norms all contain between 50 and 60 weight percent carbonate minerals. All the river norms contain halite (<20 percent) and only the South American average lacks anhydrite (all sulfates of this assemblage are alkali-bearing).

The contrast in salt norms between the average river waters and seawater but also between the river waters themselves, suggests the usefulness of the

Table 9. Salt norms (anhydrous weight percent) of representative water samples

[Salts of minor solutes, except total of nitrate salts, omitted]

Sample number		1	2	3	4	5	6	7	8	9	10
TDS (mg/L)		332*	243	229*	634*	3,641*	567*	1,323*	1,052*	148*	113*
Calcite	$CaCO_3$	88.4	53.7	-	-	-	-	0.3	2.3	17.2	7.0
Dolomite	$CaMg(CO_3)_2$	4.7	20.3	71.8	57.0	13.5	10.4	1.7	0.4	30.7	42.8
Magnesite	$MgCO_3$	-	-	1.0	0.2	72.4	65.2	-	-	-	-
Trona	$Na_3H(CO_3)_2 \cdot 2H_2O$	-	-	7.4	-	-	-	89.1	65.9	-	-
Pirssonite	$Na_2Ca(CO_3)_2$	-	-	-	-	-	-	0.6	4.7	43.3	25.1
Burkeite	$Na_6CO_3(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Anhydrite	$CaSO_4$	-	5.0	-	24.7	1.6	10.8	-	-	-	-
Kieserite	$MgSO_4 \cdot H_2O$	-	-	-	-	-	-	-	-	-	-
Thenardite	Na_2SO_4	-	-	-	-	-	-	-	-	-	-
Aphthitalite	$K_3Na(SO_4)_2$	0.2	-	1.8	-	-	-	0.5	0.4	0.2	12.1
Glauberite	$Na_2Ca(SO_4)_2$	-	14.0	-	12.6	-	-	-	-	-	-
Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	-	2.6	-	3.7	-	-	-	-	-	-
Polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$	-	-	-	-	-	-	-	-	-	-
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Kainite	$KMg(SO_4)Cl \cdot 3H_2O$	-	-	-	-	-	-	-	-	-	-
Halite	$NaCl$	5.9	4.4	-	1.1	4.6	2.2	5.0	27.5	3.7	8.3
Sylvite	KCl	0.4	-	5.3	-	-	-	1.4	0.5	1.8	1.5
Carnallite	$KMgCl_3 \cdot 6H_2O$	-	-	-	-	3.9	-	-	-	-	-
Bischofite	$MgCl_2 \cdot 6H_2O$	-	-	-	-	-	-	-	-	-	-
Tachyhydrite	$CaMg_2Cl_6 \cdot 12H_2O$	-	-	-	-	-	-	-	-	-	-
Antarcticite	$CaCl_2 \cdot 6H_2O$	-	-	-	-	-	-	-	-	-	-
Nitrate salts		-	-	-	-	3.8	9.8	-	-	-	-

*mg/kg +Epsomite ($MgSO_4 \cdot 7H_2O$) rather than kieserite. #Picromerite ($K_2Mg[SO_4]_2 \cdot 6H_2O$) rather than leonite.

1. Ground water from Tertiary Castle Hayne Limestone, New Bern, North Carolina (White and others, 1963, table 6).
2. Ground water from Lillehammer sandstone and conglomerate, SE Norway (Englund, 1983, table 1).
3. Ground water from Miocene Columbia River Basalt Group, Farmington, Oregon (White and others, 1963, table 2).
4. Ground water from Precambrian Sioux Quartzite, Sioux Falls, South Dakota (White and others, 1963, table 9).
5. Ground water from serpentine, Baltimore, Maryland (White and others, 1963, table 2).
6. Ground water from Silurian Peebles Dolomite, Bainbridge, Ohio (White and others, 1963, table 7).
7. Ground water from Homestake Mine, Lawrence Co., South Dakota (White and others, 1963, table 24).
8. Ground water from Cretaceous Benton Shale, La Prele, Wyoming (White and others, 1963, table 5).
9. Ground water from rhyolite, Mebane, North Carolina (White and others, 1963, table 1).
10. Ground water from granite, McCormack, South Dakota (White and others, 1963, table 1).

salt norm in identifing solute sources despite the lack of direct information on the geochemical evolution of the waters. Except for dilute waters deriving their principal solutes from surficial sources, major-solute categories can most readily be related to principal lithologies (Jones, 1966; Garrels, 1967; Hem, 1970; and Drever, 1982). Thus, for the major anions, carbonate waters are associated with the dissolution of limestones or silicate hydrolysis. Sulfate waters reflect the oxidation of reduced sulfur and/or the dissolution of gypsum. Chloride waters are most likely associated with an ultimate source in marine salts or hydrothermal systems, though they commonly are recycled and modified in continental basins, such as the Great Salt Lake (Spencer and others, 1985). At the same time, for the major cations, the alkalis are prominent in waters associated with siliceous crystalline rocks, pyroclastics, and the sediments derived therefrom; calcium is dominant in waters from carbonate or plagioclase-rich rocks; magnesium is characteristic of waters interacting with mafic rocks and marine muds; and all the major cations can be important in waters associated with mixed clastic lithologies. Such considerations, particularly for saline waters, can point to normative salt assemblages characteristic of genetic end members.

To test the interpretive value of the normative analysis and to establish the most diagnostic assemblages, we have computed salt norms for more than 500 analyses of fresh and saline waters from a wide variety of environments worldwide. From the final tabulations we have selected 50 examples (table 9) to illustrate a broad range of normative characteristics. Because solute derivation is most readily related to mineral reaction and tends to be of much interest in salinity problems, particular attention was given to various ground waters, seawater mixtures, and saline basin waters. In table 9, normative salt minerals are arranged according to major anion groups in order of carbonates, then sulfates, then chlorides, with mixed anion phases intermediate. Within each anion group, the sequence generally is from simple, single cation-anion phases to more complex double salts, with minor exceptions, this sytem corresponds to increasing single-phase aqueous solubility. Our attempt to reconcile increasing salt complexity with increasing solubility produces a different cation sequence for the chlorides than for the carbonates and sulfates.

We tried to choose sample salt norms for table 9 so as to have two examples with abundant amounts of each major-solute phase, some additional samples were taken from special lithologic environments or from unusual normative salt assemblages. From the results of all the salt-norm computations, a diagnostic chart has been derived (fig. 4). Although many natural waters reflect multiple solute origins, salt norms basically fall into three major categories: meteoric, marine, and diagenetic. These general

Table 9 (continued)

Sample number		11	12	13	14	15	16	17	18	19	20
TDS (mg/L)		477*	4,111*	1.023*	563*	8,710	371,700	428	905*	3,960	115
Calcite	$CaCO_3$	-	-	0.1	-	-	-	-	7.4	-	1.8
Dolomite	$CaMg(CO_3)_2$	0.9	8.7	24.6	24.3	-	-	-	4.5	5.0	22.9
Magnesite	$MgCO_3$	0.4	-	-	7.8	0.6	0.4	3.4	-	0.1	-
Trona	$Na_3H(CO_3)_2 \cdot 2H_2O$	60.2	15.1	-	-	-	-	-	-	-	-
Pirssonite	$Na_2Ca(CO_3)_2$	-	6.3	-	-	-	-	-	-	-	-
Burkeite	$Na_6CO_3(SO_4)_2$	31.4	30.2	-	-	-	-	-	-	1.5	-
Anhydrite	$CaSO_4$	-	-	70.6	56.8	3.0	1.7	40.8	-	-	8.9
Kieserite	$MgSO_4 \cdot H_2O$	-	-	-	-	35.8	76.6	28.6+	-	-	-
Thenardite	Na_2SO_4	-	-	-	-	-	-	-	52.9	45.6	-
Aphthitalite	$K_3Na(SO_4)_2$	0.3	5.1	-	-	-	-	-	-	0.5	-
Glauberite	$Na_2Ca(SO_4)_2$	-	-	-	6.2	-	-	-	24.9	-	46.0
Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	-	-	-	4.0	-	-	-	4.7	-	8.8
Polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$	-	-	-	-	2.4	-	4.5	-	-	-
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	18.8	-	-	-
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Kainite	$KMg(SO_4)Cl \cdot 3H_2O$	-	-	-	-	-	-	-	-	-	-
Halite	$NaCl$	6.5	33.2	3.5	0.6	55.2	13.2	3.7	4.7	46.6	11.3
Sylvite	KCl	-	-	0.3	-	-	-	-	-	-	-
Carnallite	$KMgCl_3 \cdot 6H_2O$	-	-	0.7	-	2.9	7.7	-	-	-	-
Bischofite	$MgCl_2 \cdot 6H_2O$	-	-	-	-	-	0.4	-	-	-	-
Tachyhydrite	$CaMg_2Cl_6 \cdot 12H_2O$	-	-	-	-	-	-	-	-	-	-
Antarcticite	$CaCl_2 \cdot 6H_2O$	-	-	-	-	-	-	-	-	-	-
Nitrate salts		-	-	-	-	-	-	-	-	-	-

*mg/kg +Epsomite ($MgSO_4 \cdot 7H_2O$) rather than kieserite. #Picromerite ($K_2Mg[SO_4]_2 \cdot 6H_2O$) rather than leonite.

11. Ground water from lower Mesozoic Navajo Sandstone, Mexican Water, Arizona (White and others, 1963, table 4).
12. Doughty Springs, Delta Co., Colorado (White and others, 1963, table 23).
13. Ground water from Silurian Camillus and Vernon Shales, Syracuse, New York (White and others, 1963, table 5).
14. Ground water from Mississippian Pahasapa Limestone, Rapid City, South Dakota (White and others, 1963, table 6).
15. Interstitial brine #47, Chott el Jerid, Tunisia (Gueddari and others, 1983, table 1).
16. Surficial brine LS10 from Salicor playa, LaMancha region, Spain (Soriano and others, 1977, table 1).
17. Ground water from Sudbury area, Ontario, Canada (Frape and others, 1984, table 1).
18. Ground water in Paleozoic granite from Chester, Virginia (White and others, 1963, table 1).
19. Ground water from Enoch's Pond well, Bailey Co., Texas (Chemerys, J. C. and Wood, W. W., pers. commun.).
20. Ground water from Sudbury area, Ontario, Canada (Frape and others, 1984, table 1).

Table 9 (continued)

Sample number		21	22	23	24	25	26	27	28	29	30
TDS (mg/L)		1,107*	1,886*	475*	3,264 -	324,7*	339,300	239,200	643*	82	1,713
Calcite	$CaCO_3$	-	-	34.8	-	-	-	-	-	1.7	-
Dolomite	$CaMg(CO_3)_2$	15.6	32.4	11.5	-	-	-	-	39.1	23.2	-
Magnesite	$MgCO_3$	10.9	0.2	-	2.9	2.3	0.07	0.1	-	-	8.0
Trona	$Na_3H(CO_3)_2 \cdot 2H_2O$	-	-	-	-	-	-	-	4.4	-	-
Pirssonite	$Na_2Ca(CO_3)_2$	-	-	-	-	-	-	-	15.1	-	-
Burkeite	$Na_6CO_3(SO_4)_2$	-	-	-	-	-	-	-	17.6	-	-
Anhydrite	$CaSO_4$	-	23.9	24.4	1.8	31.8	-	-	-	-	31.4
Kieserite	$MgSO_4 \cdot H_2O$	-	-	-	-	-	-	4.4$^+$	-	-	7.5
Thenardite	Na_2SO_4	3.7	-	-	-	-	-	-	-	4.2	-
Aphthitalite	$K_3Na(SO_4)_2$	-	-	-	-	-	0.2	-	19.2	18.7	-
Glauberite	$Na_2Ca(SO_4)_2$	64.7	5.3	15.8	-	21.5	-	-	-	21.3	-
Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	-	17.4	10.8	2.7	-	-	-	-	-	-
Polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$	-	-	-	61.5	3.1	0.2	1.6	-	-	7.5
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	39.3	37.6	0.8	-	-	-
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	9.2$^\#$	7.1	-	-	-
Kainite	$KMg(SO_4)Cl \cdot 3H_2O$	-	-	-	-	-	-	-	-	-	-
Halite	$NaCl$	1.1	17.8	2.3	31.2	2.0	52.7	86.1	3.5	30.8	41.8
Sylvite	KCl	-	-	-	0.03	-	-	-	-	-	-
Carnallite	$KMgCl_3 \cdot 6H_2O$	-	-	-	-	-	-	-	-	-	3.5
Bischofite	$MgCl_2 \cdot 6H_2O$	-	-	-	-	-	-	-	-	-	-
Tachyhydrite	$CaMg_2Cl_6 \cdot 12H_2O$	-	-	-	-	-	-	-	-	-	-
Antarcticite	$CaCl_2 \cdot 6H_2O$	-	-	-	-	-	-	-	-	-	-
Nitrate salts		-	-	-	-	-	-	-	1.0	-	-

*mg/kg $^+$Epsomite ($MgSO_4 \cdot 7H_2O$) rather than kieserite. $^\#$Picromerite ($K_2Mg[SO_4]_2 \cdot 6H_2O$) rather than leonite.

21. Ground water from glacial deposits, Malcolm, Iowa (White and others, 1963, table 11).
22. Mammoth Springs, Yellowstone Park, Wyoming (White and others, 1963, table 25).
23. Ground water from Precambrian Siamo Slate, Morris Mine, Minnesota (White and others, 1963, table 10).
24. Interstitial fluid #20, Chott el Jerid, Tunisia (Gueddari and others, 1983, table 1).
25. Ground water from Cretaceous Pierre Shale, Langdon, North Dakota (White and others, 1963, table 5).
26. Salt Lake, Roosevelt Co., New Mexico (Chemerys, J. C. and Wood, W. W., pers. commun.).
27. Interstitial brine sample 47-27-022, Salt Lake playa, Hudspeth Co., Texas (Boyd, 1982, table 7).
28. Ground water from gabbro, Waterloo, Maryland (White and others, 1963, table 2).
29. Ground water from morraine, Moss area, SE Norway (Englund and Myhrstad, 1980, table 1).
30. Deep well, Ouargla Oasis #3, Tunisia (Clarke and Jones, 1972, table 2).

Table 9 (continued)

Sample number		31	32	33	34	35	36	37	38	39	40
TDS (mg/L)		103,800	135,700	331,200	310,900	389,200	253,300*	266,400	907	4,308	271,300
Calcite	$CaCO_3$	-	-	-	-	-	0.2	-	-	-	-
Dolomite	$CaMg(CO_3)_2$	-	-	-	-	-	-	-	3.4	-	0.08
Magnesite	$MgCO_3$	0.3	-	-	0.02	-	-	0.02	-	2.1	-
Trona	$Na_3H(CO_3)_2 \cdot 2H_2O$	-	-	-	-	-	-	-	-	-	-
Pirssonite	$Na_2Ca(CO_3)_2$	-	-	-	-	-	-	-	-	-	-
Burkeite	$Na_6CO_3(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Anhydrite	$CaSO_4$	-	0.04	1.1	1.6	-	<0.01	0.5	31.1	28.5	0.2
Kieserite	$MgSO_4 \cdot H_2O$	6.9	-	-	0.07	-	-	5.2	-	3.7	-
Thenardite	Na_2SO_4	-	-	-	-	-	-	-	-	-	-
Aphthitalite	$K_3Na(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Glauberite	$Na_2Ca(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	-	-	-	-	-	-	-	-	-	-
Polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$	7.4	-	-	0.2	-	-	-	-	-	-
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Kainite	$KMg(SO_4)Cl \cdot 3H_2O$	1.9	-	-	-	-	-	-	-	-	-
Halite	$NaCl$	80.2	84.3	97.9	97.4	48.1	52.7	80.2	30.8	45.5	48.7
Sylvite	KCl	-	-	0.02	0.8	15.9	13.6	-	-	-	-
Carnallite	$KMgCl_3 \cdot 6H_2O$	3.3	1.0	0.1	0.8	25.4	0.2	12.3	7.7	3.5	7.2
Bischofite	$MgCl_2 \cdot 6H_2O$	-	-	-	-	-	-	1.8	24.8	16.8	-
Tachyhydrite	$CaMg_2Cl_6 \cdot 12H_2O$	-	2.1	-	-	-	-	-	2.2	-	43.7
Antarcticite	$CaCl_2 \cdot 6H_2O$	-	12.2	0.7	-	9.2	31.1	-	-	-	0.05
Nitrate salts		-	-	-	-	-	-	-	-	-	-

*mg/kg +Epsomite ($MgSO_4 \cdot 7H_2O$) rather than kieserite. #Picromerite ($K_2Mg[SO_4]_2 \cdot 6H_2O$) rather than leonite.

31. Interstitial brine sample 48-24-021, Salt Lake basin playa, Hudspeth Co., Texas (Boyd, 1982, table 7).
32. Average of 40 formation waters, Louisiana Gulf Coast (Dickey and others, 1972).
33. Sample AV12, seepage in Avery Island salt dome, Louisiana (Kumar, 1983, table 2).
34. Caspian Gates Spring, Shiraz basin, Iran (Zak and Gat, 1975, table 1).
35. Sample AV36, seepage in Avery Island salt dome, Louisiana (Kumar, 1983, table 2).
36. Salton Sea geothermal well, I.I.D. no. 1, California (White, 1968, table 1).
37. Interstitial fluid #111, Chott el Jerid, Tunisia (Gueddari and others, 1983, table 1).
38. Corral Rubio playa LP31, LaMancha region, Spain (Marfil and others, 1975, table 4).
39. Feiran well #9, southern Sinai desert (Starinsky and others, 1983, table 2).
40. Formation water from well Zohar #6, Sherif Fm., Jurassic, southern Israel (Fleischer and others, 1977, table 1).

Table 9 (continued)

Sample number		41	42	43	44	45	46	47	48	49	50
TDS (mg/L)		363,400	241,000	400,300	510	72*	898	534	252	709	1,472*
Calcite	$CaCO_3$	-	-	-	10.5			36.2			
Dolomite	$CaMg(CO_3)_2$	0.2	-	-	26.0	5.2	0.3	21.8	6.6	39.7	-
Magnesite	$MgCO_3$	-	-	-	-	21.8	-	-	-	-	6.8
Trona	$Na_3H(CO_3)_2 \cdot 2H_2O$	-	-	-	-	-	-	-	-	-	-
Pirssonite	$Na_2Ca(CO_3)_2$	-	-	-	-	-	-	-	-	-	-
Burkeite	$Na_6CO_3(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Anhydrite	$CaSO_4$	<0.01	0.08	0.01	23.4	26.0	10.4	29.9	6.2	23.2	36.3
Kieserite	$MgSO_4 \cdot H_2O$	-	-	-	-	-	-	-	-	-	5.2
Thenardite	Na_2SO_4	-	-	-	-	-	-	-	-	-	-
Aphthitalite	$K_3Na(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Glauberite	$Na_2Ca(SO_4)_2$	-	-	-	-	-	-	-	-	-	-
Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	-	-	-	-	-	-	-	-	-	-
Polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$	-	-	-	-	-	-	-	-	-	-
Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	-	-	-	-	-	-	-	-	-	-
Kainite	$KMg(SO_4)Cl \cdot 3H_2O$	-	-	-	-	-	-	-	-	-	-
Halite	$NaCl$	4.3	19.0	19.0	33.0	20.0	66.3	9.4	8304	27.0	40.9
Sylvite	KCl	-	0.09	-	-	-	-	0.4	-	-	-
Carnallite	$KMgCl_3 \cdot 6H_2O$	23.0	0.03	10.0	1.7	9.9	5.3	2.3	1.5	0.9	4.5
Bischofite	$MgCl_2 \cdot 6H_2O$	-	-	-	-	-	-	-	-	4.0	3.8
Tachyhydrite	$CaMg_2Cl_6 \cdot 12H_2O$	48.0	-	17.0	-	-	3.4	-	2.5	0.4	-
Antarcticite	$CaCl_2 \cdot 6H_2O$	22.8	79.7	53.0	5.2	-	14.2	-	2.5	-	-
Nitrate salts		-	-	-	-	14.1	-	-	-	4.8	2.3

*mg/kg +Epsomite ($MgSO_4 \cdot 7H_2O$) rather than kieserite. #Picromerite ($K_2Mg[SO_4]_2 \cdot 6H_2O$) rather than leonite.

41. Oil field brine, Delhi-Taylor #2, Seven Mile Fm., Grand Co., Utah (Mayhew and Heylmun, 1965, no. 4).
42. Waters from North Mine, Sudbury district, Ontario, Canada (Frape and Fritz, 1982, table 1).
43. Oil field brine, Silurian Niagaran Series, Ingham Co., Michigan (Carpenter, 1979, table 5).
44. Ground water from granite, well D647, SW Sinai area (Gat and Issar, 1974, table 2).
45. Ground water from Precambrian Baltimore Gneiss, Bucks Co., Pennsylvania (White and others, 1963, table 10).
46. Ground water from gneiss and amphibolite, As, Moss areas, SE Norway (Englund, 1983, table 1).
47. Ground water from Grimsby area, NE England (Howard and Lloyd, 1983, table 3).
48. Ground water from Quaternary marine deposits, SE Norway (Englund, 1983, table 1).
49. Ground water from Cambrian Conasauga Limestone, Birmingham, Alabama (White and others, 1963, table 6).
50. Deep well, Rahmat 2, Tunisia (Clarke and Jones, 1972, table 2).

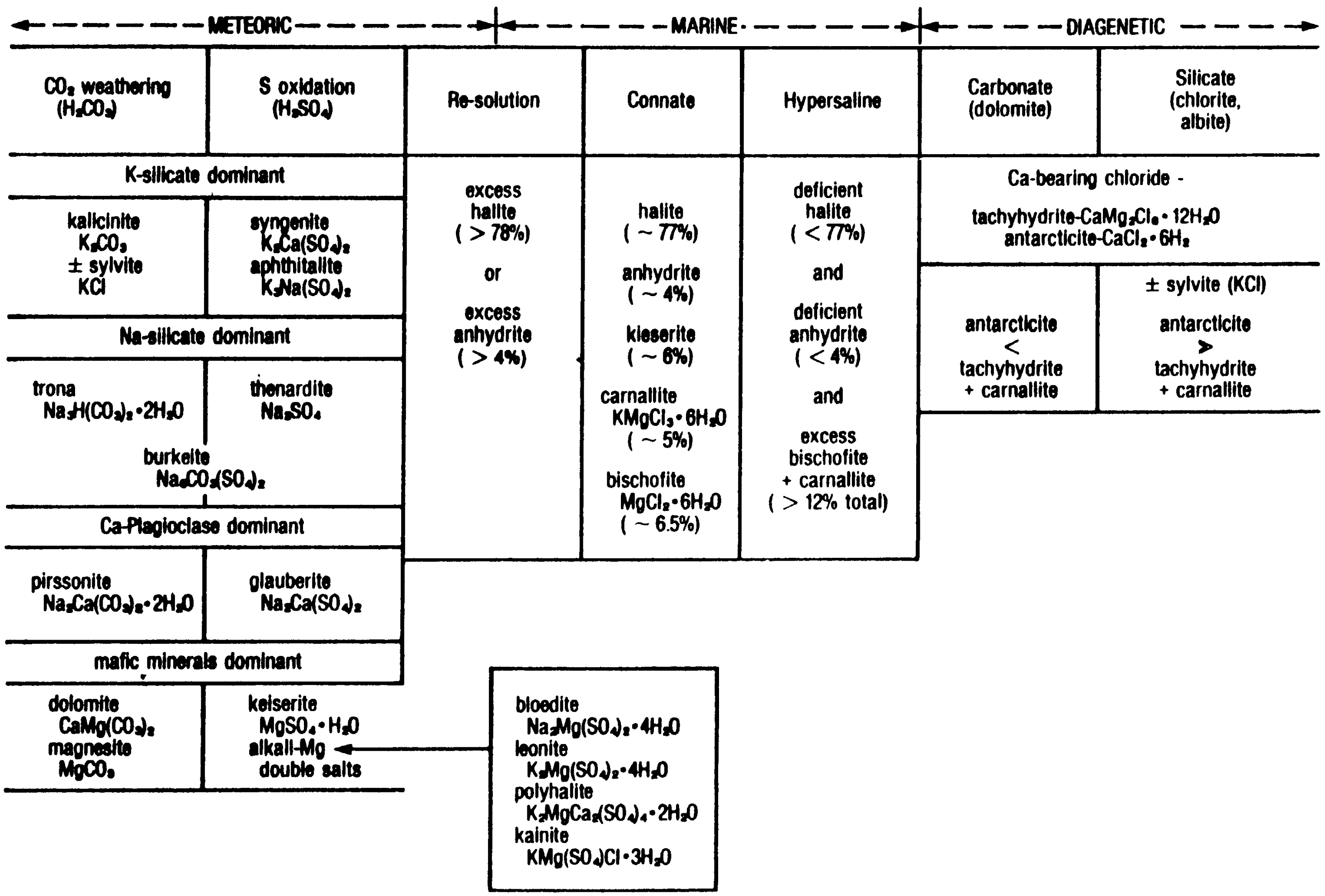

Figure 4. Diagnostic chart for normative salts. Major categories of meteoric, marine, or diagenetic assemblages are further subdivided according to principal agent or lithologic environment of solute derivation in terms of diagnostic individual salts, assemblages, or abundances.

categories are based on qualitative similarity of complete normative assemblages rather than on detailed characteristics of the constituent phases.

Meteoric Norms

Salt norms for meteoric water deriving their solutes principally from rock weathering reflect the principal agent promoting dissolution in the pedogenic environment. In addition to direct aqueous dissolution of mineral salts, such as the carbonate minerals, carbonic acid and sulfuric acid in meteoric waters each generate their characteristic solute compositions. A distinctive feature of the normative assemblages from meteoric waters is the absence of the alkaline-earth-bearing chlorides.

Carbonic acid hydrolysis of rock-forming minerals produces a salt norm dominated by carbonate minerals (table 9). The very high calcite abundance in the norm from the Tertiary Castle Hayne Limestone (#1) of North Carolina or the calcic Permian clastics of SE. Norway (#2), and the abundant normative dolomite in waters from the Mississippian Pahapsa Limestone of South Dakota (#14) and the Cambrian Conasuaga Limestone of Alabama (#49) are examples of straight forward cabonate-rock dissolution. The occurrence of normative alkali carbonate phases (trona or kalicinite), on the other hand, is diagnostic of silicate hydrolysis. Examples of silicate hydrolysis are given in table 9 in the trona-bearing salt norms for ground waters from siliceous crystalline or clastic rocks, for example, the granite of the Black Hills, South Dakota (#7), the Cretaceous Benton Shale of Wyoming (#8), or the lower Mesozoic Navajo sandstone, Arizona (#11).

In the absence of carbonate rock dissolution, contrasts in amounts of trona, alkali alkaline-earth double carbonate (pirssonite), and alkaline-earth carbonate in the norm reflect variations in the alkali/alkaline-earth ratios in silicate minerals (feldspar and pyroxene or amphibole) in the associated lithologies. Increased importance of Ca-plagioclase and/or mafic minerals is reflected in the norms for ground water from the granite of McCormack, South Carolina (table 9, #10), or metamorphosed volcanic rocks at Mebane, North Carolina (table 9, #9). The norms for waters associated with normal carbonic acid weathering of mixed alkali-bearing silicate rocks commonly contain sylvite (table 9, #3, 7, 8, 9, 10). The lower solubility of the trona-sylvite pair compared to that of the kalicinite-halite pair under atmospheric conditions leaves potassium associated with chloride in the normative calculation. Normative kalicinite appears only in salt norms for ground waters where potash feldspar is the dominant solute source. Large amounts of normative dolomite can result from hydrolysis of mixed Ca-Mg silicates, such as the plagioclase-pyroxene mineralogy of basalt or gabbro (table 9, #3 and 28). Abundant normative magnesite, on the other hand, requires hydrolysis of dominantly magnesium silicate, such as serpentine (table 9, #5), biotite (table 9, #45), or even Mg clays in carbonate rock (table 9, #6).

Meteroic waters aided in weathering by sulfuric acid derived from the oxidation of sulfides (perhaps cycling through acid rain; table 9, #2 and #29) produce salt norms characterized by sulfate minerals. Predominant anhydrite in the norm can, of course, simply reflect dissolution of original evaporitic $CaSO_4$, such as in waters from the Silurian gypsiferous red beds of central New York (table 9, #13) and the gypsiferous Pahasapa Limestone of South Dakota (#14). In addition, abundant normative potassium-magnesium-mixed sulfates can be characteristic of residual meteoric fluids following fractional precipitation of gypsum and/or carbonates (table 9, #27 and #31).

The presence of either of the pure alkali sulfates, thenardite (Na_2SO_4) and aphthitalite ($K_3Na(SO_4)_2$), or of the alkali sulfo-carbonate, burkeite ($Na_6CO_3(SO_4)_2$), or of the alkali-calcium double salts, glauberite ($Na_2Ca(SO_4)_2$) and syngenite ($K_2Ca(SO_4)_2 \cdot 2H_2O$) can be considered diagnostic of sulfatic-weathering solutions. The former can be expected from waters associated with the weathering of siliceous crystalline rocks and their clastic derivatives, whereas, the glauberite and syngenite reflect more calcic lithologies. Solute magnesium derived from sulfuric-acid hydrolysis of mafic lithologies may appear in salt norms as the monohydrate sulfate, keiserite, or its more hydrous equivalent, epsomite. Usually, however, the magnesian component of hydrolysis appears in the salt norm as dolomite or as the alkali-bearing complex salts bloedite ($Na_2Mg(SO_4)_2$), polyhalite ($K_2MgCa(SO_4)_3$), leonite ($K_2Mg(SO_4)_2 \cdot 4H_2O$), or kainite ($KMg(SO_4)Cl \cdot 3H_2O$). The occurrence of such sulfates in the salt norm indicates sulfuric-acid hydrolysis of mixed-mafic silicate, either from crystalline rocks (table 9, #17) or fine clastic sediments (table 9, #25). Examples of sulfate-rich norms spanning the whole range of crystalline and clastic lithologies are given in table 9 for waters associated with granite in Virginia (#18), granitic basement derived glacial deposits in Iowa (#21) or gabbro at Waterloo, Maryland (#28), basic plutonic rocks at Sudbury, Ontario(#17), and calcic micaceous slate from northern Michigan (#23).

Marine Norms

Seawater-type norms dominated by sulfate and chloride salts are particularly characterized by magnesium-associated chloride. This association cannot be obtained from hydrothermal sources because of the aqueous insolubility of Mg-silicates at elevated temperature. Such an association in the salt norm from other than ultimately marine sources would require dissolution of chloride-bearing mafic minerals.

Normative diagnosis of marine solute sources is complicated not only by mixing or continental recycling, but also by solute redistribution within and marginal to the marine environment. Three subdivisions can readily be recognized: connate, resolution, and hypersaline. These categories are based on abundance, as well as the presence or absence of key phases in the salt norm. Thus, any unaltered connate seawater dilution or dilution therof should give the seawater salt norm (table 8) with the characteristic assemblage halite-anhydrite-kieserite-carnallite-bischofite in the proportions given (as also shown in fig. 4). A solute matrix derived from resolution of the most common evaporite minerals, halite and gypsum, is derived in the same way as other meteoric waters; the matrix will be enriched in NaCl and $CaSO_4$ and depleted in the other constituents. In contrast, the solutes of a hypersaline marine bittern will be depleted in NaCl and $CaSO_4$ because of fractional precipitation of those salts, but the salt norm will include excess magnesium and, most likely, potassium-bearing chloride salts. This is because the molar ratio of chloride to sodium in seawater is greater than unity (the molar value is 1.17), so that the next most abundant cations, Mg and K, both appear as chlorides in the salt norm. Changes in proportions of the major normative salts corresponding to the evaporative concentration of seawater are given in table 10, as calculated from the analyses of hypersaline liquors in coastal marine-salt evaporation ponds.

Of all the samples for which salt norms were calculated, only a few computations produced results similar to those expected for dilution of connate seawater. This is expected, as mixing, continental recycling, or mineral-water interaction of any sort should produce differences from seawater proportions. Because of the relative stabilities of the minerals considered by SNORM, additions of calcium, carbonate, or sulfate to a seawater solute matrix will appear in the salt norm as excess magnesite and anhydrite; this also can eliminate bischofite and introduce sylvite into the norm as Mg becomes associated with carbonate or sulfate rather than with chloride. Additions of sodium will be seen as NaCl, with an associated redistribution of other mineral proportions, depending on the accompanying anion. Thus, an excess of magnesite, anhydrite, or halite over that in the seawater norm appears indicative of mixing with meteoric solutions or continental cycling. The effects of marine aerosols may be seen in the dilute waters of some areas subject to coastal precipitation patterns (table 9, #45 and #47).

The waters that most closely approach the seawater norm are from the continental saline basins of northern Algeria (table 9, Chott el Jerid, #37) and western Australia (table 11). The former has an overall excess of chlorides and a deficiency of sulfate, indicating hypersaline conditions. However, the halite compared to the seawater norm suggests some resolution as well. The Yilgarn examples include (1) groundwater norms with definite,

Table 10. Salinity, major anion concentration, and salt norms for hypersaline marine liquors from surface evaporation ponds

[Abbreviations of normative phase names from table 2]

Sample	-----Concentration (mg/kg)-----			E_{Br}[#]	Salt norm[*] (anhydrous weight percent)				
	Salinity	Chloride	Sulfate		hal	anh	kie	car	bis
Black Sea ponds, Ukraine (Zherebtsova and Volkova, 1966)									
gypsum ppt.	170,000	95,310	11,760	5.9	79.0	1.8	7.1	5.0	7.1
halite ppt.	270,000	149,400	22,580	15.0	71.5	0.3	10.3	7.25	10.7
Mg-sulfate ppt.	309,200	148,100	63,920	44.2	30.8	-	26.1	19.3	23.7
K-salt ppt.	314,600	173,600	43,490	71.0	13.8	-	17.5	27.7	40.9
>K-salt ppt.	329,800	192,700	41,120	90.2	5.2	-	15.8	18.7	60.2
Portoroz salt ponds (Herrmann and others, 1973)									
pan 12	137,300	76,800	10,130	3.8	77.1	3.2	6.4	4.8	8.2
pan 13c	252,200	143,900	15,600	7.1	78.7	0.6	7.2	5.0	8.2
pan 13e	274,100	151,100	29,900	12.5	61.0	0.2	13.4	7.7	17.3
pan 13h	273,100	149,000	33,000	15.8	51.2	0.2	15.0	10.2	23.0

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[*] Normative carbonate salts not reported; aqueous carbonate species negligible (Portoroz) or not reported (Black Sea).

[#] Degree of evaporation of brine compared to normal seawater (after Levy, 1977) based on relative Br content; value a minimum beyond halite saturation because of neglect of Br uptake by chloride salts.

Table 11. Salt norms for selected analyses of groundwaters from the salt lake areas of the Yilgarn Block, Western Australia; samples chosen from data of Mann (1983) to illustrate complete compositional range in normative marine salts and are presented in order of increasing halite

[Abbreviations of normative phase names from table 2]

Sample	Location (part of block)	Salinity (mg/L)	Salt norm (anhydrous weight percent)									
			hal	anh	mag	kie	pol	leo	blo	kai	car	bis
Marine assemblages												
500	SW corner	323,300	71.9	0.3	<0.1	8.4	-	-	-	-	2.2	17.1
518	WSW edge	147,100	74.6	3.0	<0.1	5.0	-	-	-	-	2.0	15.4
62	N. edge	48,200	77.0	5.9	0.1	12.0	-	-	-	-	3.1	1.8
70	NNW edge	23,600	77.8	15.5	0.4	3.7	1.0	-	-	-	1.6	-
506	S. part	142,300	81.2	0.9	<0.1	5.4	-	-	-	-	4.5	5.9
509	S. edge	217,200	83.2	1.8	-	2.9	-	-	-	-	3.7	8.4
393	center	151,900	84.6	2.9	<0.1	4.2	-	-	-	-	0.6	7.5
403	W. part	153,200	85.5	3.5	<0.1	3.3	-	-	-	-	4.8	2.8
399	N. central	230,900	91.0	1.0	<0.1	4.0	-	-	-	-	2.9	1.0
Mixed marine-meteoric assemblages												
65	N. part	21,840	81.3	-	0.9	9.1*	6.5	1.5	0.7	-	-	-
243	NE edge	22,700	88.7	-	<0.1	4.7*	2.2	2.5	-	1.8	-	-

*Normative epsomite rather than kieserite.

though small, deficiencies of halite and anhydrite along with sufficient bischofite; these salts indicate clear hypersaline affinities (table 11, #500 and #518), and (2) surface water with normative proportions about as close to seawater as might be imagined in continental environs. Most of the Yilgarn salt norms, however, show a telltale excess of halite resulting from resolution. In fact, the majority of the Yilgarn salt norms (table 11) produce enough excess halite to suggest recycling of marine solutes with little contribution from direct weathering of the granitic crystalline basement of the region (unless dominated by chloride-bearing mafic minerals). However, the normative salt abundances for some Yilgarn samples (table 11, #65 and #243) and most other closed basin waters can be interpreted as the result of mixing of meteoric weathering solutions with a recycled marine-solute matrix. Well water from the north Sahara produced a complete seawater assemblage in the salt norm (table 9, #50) but with halite and bischofite quantities much reduced and anhydrite and magnesite increased over a seawater norm primarily because of addition of sulfate and carbonate solutes from continental sources. Similarly, well water of the southern Sinai (table 9, #39), is deficient in normative halite and has an excess of magnesium chloride suggesting a hypersaline solute origin as supported by strontium-isotope evidence (Starinsky and others, 1983). Excess normative anhydrite and magnesite, however, suggest additional (meteroic) solute contributions.

A key normative mineral indicator of meteoric additions to a marine-type, sulfo-chloride anion matrix is the unusual mineral, kainite $KMg(SO_4)Cl \cdot 3H_2O$. This phase appears in the norms of samples from the edge of the Yilgarn block (table 11, #243) and from the Salt Lake playa of West Texas (table 9, #31), which has derived the bulk of its solutes from weathering of the evaporitic Permian strata of the area. These salt norms represent the addition of excess sulfate to a marine solute matrix, while the proportions of alkalies and Mg were maintained.

A less diagnostic mineral commonly appearing in salt norms for modified marine waters is sylvite. If a water containing alkaline-earth or sodium chloride is mixed with a water containing potassium sulfo-carbonate from weathering, the salt norm calculation will associate the carbonate and sulfate with the other cations. After consuming available Mg in polyhalite, kainite, or carnallite, KCl is left as a distinct phase. Mixing of any other type of water with a residual marine bittern merely increases the likelihood of sylvite occurring as a single phase in the salt norm. Thus, additional information besides the presence of sylvite in the norm is needed to suggest solute affinities. The appearance of sylvite in normative alkali sulfo-carbonate assemblages attests to its compatibility with weathering solutions; however, its presence within other chloride-dominant normative assemblages bespeaks its involvement in different phenomena, which will be discussed below.

Another normative mineral that can serve as an indicator of mixing of weathering solutions with a seawater-type solute matrix is kieserite. The abundance of normative kieserite can be reduced by addition of redissolved halite and/or calcium sulfate. Normative kieserite is increased in a solute matrix with additions of sulfate from weathering, regardless of whether subsequent sequential evaporative precipitation of $CaSO_4$ and/or NaCl occurs (table 9, #15 and #16). The addition of dilute calcium sulfo-carbonate solutes typical of meteoric waters to oxic, gypsum-saturated, hypersaline fluids also will deplete normative kieserite through loss of sulfate with calcium and of magnesium with carbonate (the latter will also result from sulfate reduction). Without the low values for activity of water generated by coexistant hydroscopic chlorides, kieserite is unstable relative to its more hydrous equivalent, epsomite ($MgSO_4 \cdot 7H_2O$; table 9, #27). Kieserite occurs in the norm of all but 4 of 48 analyses from the Yilgarn block, western Australia (table 11).

Waters illustrating the extreme proportions of solute NaCl that can result from halite resolution in the subsurface include a salt dome mine seepage (table 9, #33) and a surface spring associated with a shallow subsurface dome (#34). The clear indication that excess halite from salt resolution predominates over solute diagenesis, as suggested by Hanor (1984), also is indicated in the salt norm for the average of 40 formation waters from the Louisiana Gulf Coast (table 9, #32).

The chloride minerals characteristic of hypersaline marine fluids and similar continental and modified sedimentary basin brines, as well, are bischofite ($MgCl_2 \cdot 6H_2O$) and the K-Mg double halide, carnallite ($KMgCl_3 \cdot 6H_2O$). Small quantities of these minerals also appear in the norm of relatively dilute ground waters associated with diverse rock types, suggesting the presence of seawater-type solutes and possibly aerosols; in ground waters from coastal sediments (table 9, #47), the latter is most likely the case. Ground waters in crystalline rock terranes of the United States, Canada, and Scandanavia (table 9, #5, #45, and #46), however, may contain solutes of diagenetic origin. Substantial normative amounts of bischofite. carnallite, and/or sylvite are computed for brines of clearly saline strata or dilutions thereof (table 9, #35, #37, #38, #39, and #41). Normative abundance of carnallite and bischofite more than the amounts found in the seawater norm appear to be clearly associated with hypersaline waters.

Diagenetic Norms

The calcium-bearing chloride minerals, antarcticite ($CaCl_2 \cdot 6H_2O$) and tachyhydrite ($CaMg_2Cl_6 \cdot 12H_2O$), indicate solute diagenesis and the highly altered fluid compositions with respect to earth-surface conditons. Yet, calcium chloride-bearing normative assemblages were computed for a number of analyses representing diverse conditions. Nearly all such salt norms were obtained from subsurface fluids associated with deep sedimentary basins, highly saline strata, or crystalline shield areas (table 9, #32-33, #35-36, #40-44, and #46). Notable exceptions occur in a few salt norms from coastal marine sediments (table 9, #48). Assemblages containing calcium-bearing chlorides are most readily interpreted in terms of the diagenetic alteration of a residual marine-solute matrix dominated by magnesium salts through exchange of Mg and Na in solution for Ca in solids--that is, carbonate, clay minerals, or feldspar. Such exchange in silicates is promoted by elevated temperature through decrease in the solubility of magnesium silicate phases. The resulting fluid can be expected to produce an antarcticite-sylvite norm (table 9, #36). The blending of marine bittern with a deep sedimentary basin brine or hydrothermal fluid is the process postulated by Knauth and others (1980) for the Louisiana salt dome brines. Addition of exchanged solute calcium to a marine bittern would all but eliminate sulfate from the fluid by precipitation of anhydrite. In variable proportions, exchange of other ions for calcium is characteristic of all the most concentrated solutions encountered in the subsurface.

Diagenetic salt norms can apparently be subdivided on the basis of the phase ratios of calcium chloride to magnesium chloride. The development of calcium chloride brines in the Bardawil Lagoon area of north Sinai by evaporative concentration, by mixing with shallow meteoric ground waters, and by dolomitization of carbonate sediments has been documented by Levy (1977). Salt norms for representative analyses from the Bardawil Lagoon are given in table 12. In no instance does the Ca/Mg concentration (or salt norm antarcticite/tachyhydrite) ratio exceed unity. However, the decreasing ratio of activity coefficients for Ca/Mg with increasing fluid concentration permits an increasing molar Ca/Mg ratio in equilibrium with dolomite. The ratio to be found in many natural solutions, however, will differ with respect to the solute matrix and the structural state of the Ca and Mg carbonates. Although it is impossible to determine an exact limit for Ca/Mg above which dolomitization alone cannot account for the relative normative abundances, the ratio probably is from 4 to 5 (Stoessel and Moore, 1984).

Very large ratios of normative antarcticite to magnesium chloride salt ratios clearly are associated with silicate authigenesis--most specifically,

Table 12. Salt norms for representative brines from sabkhas south of the Bardawil Lagoon, north Sinai (data from Levy, 1977); samples listed according to increasingly greater distance from normal Meditteranean seawaters of the principal lagoon

[Abbreviations of normative phase names from table 2]

Sample	Sabkha	Salinity (mg/kg)	E_{Mg}*	Salt norm (anhydrous weight percent)								
				hal	anh	mag	dol	kie	car	bis	tac	ant
1083	Hawash N.	135,800	3.7	79.8	5.7	0.07	-	5.7	5.4	6.2	-	-
1082	Hawash N.	280,900	7.9	81.0	1.1	0.06	-	5.7	5.4	6.7	-	-
1083A	Hawash S.	278,700	13.2	70.2	0.8	0.09	-	8.0	6.5	14.3	-	-
1107	Hafiordim	271,400	4.5	88.3	1.0	0.02	-	3.0	3.3	4.3	-	-
1120	Hafiordim	270,000	5.8	86.7	0.8	0.01	-	0.7	4.3	7.5	-	-
1144	Hagvaot N.	269,300	8.1	80.6	0.5	0.03	-	5.2	4.9	8.8	-	-
1114	Hagvaot S.	271,700	6.1	85.6	1.8	0.02	-	0.3	2.6	9.7	-	-
1166	Hagvaot S.	262,700	16.1	63.9	1.3	-	0.04	-	5.9	25.7	3.2	-
1111	Hayareah	260,700	5.0	82.0	0.4	-	0.01	-	0.5	-	15.2	1.8
1113	Hayareah	100,900	3.6	59.5	2.1	-	0.04	-	0.5	-	28.5	9.4
1160	Hayareah	275,500	20.2	35.0	0.2	-	0.02	-	0.1	-	58.9	5.8

*Degree of evaporation of brine compared to normal seawater (after Levy, 1977) based on relative Mg content; computation neglects loss of Mg to diagenetic reactions reflected in normative occurrence of $CaCl_2$ phases.

the formation of chlorite and albite. The best examples in table 9 are in the crystalline shield brine from Canada (#42) and the sedimentary basin brine of Michigan (#43). Additions of minor amounts of these solute matrices to alkali carbonate or sulfate-bearing waters can readily obliterate the $CaCl_2$ signature (as perhaps in table 9, #39 and #45), but salt norm examples are found where small amounts of antarcticite suggest such a contribution (table 9, #44 and #46). Although calcium is usually strongly preferred on clay-mineral cation exchange sites, the possibility of displacing some calcium to the solution by high solute concentrations of other cations must, however, be considered.

Summary

Examination of more than 500 salt norms calculated from water analyses representing a wide range of concentrations and hydrochemical settings has suggested that certain key phases or assemblages are characteristic of solute origin. In addition, it appears that the interpretation of the salt norm can depend on the relative abundance of diagnostic phases, as well as their presence or absence. Normative assemblages calculated by SNORM seem to fall into three major categories: meteoric, marine, or diagenetic. Although the presence of alkali-bearing carbonates and sulfates in the salt norm seems to distinguish meteoric waters and their pricipal supplemental weathering agent, differentiation of types of marine or diagenetic fluids requires comparison of relative abundances of normative salts. Salt norms of resolution, connate, or hypersaline fluids of marine or continental recycled seawater type are distinguished by the relative amounts of halite, anhydrite and Mg-bearing chlorides, whereas different principal diagenetic processes operating on subsurface fluids are reflected in alkaline-earth chloride ratios. Although the detailed criteria have been based on the most indicative data sets known to the authors, the tests thusfar have hardly been exhaustive.

REFERENCES

Al Droubi, Abdallah, Fritz, Bertrand, Gac, Jaques-Ives, and Tardy, Yves, 1980, Generalized residual alkalinity concept; application to prediction of the chemical evolution of natural waters by evaporation: American Journal of Science, v. 280, p. 560-572.

Bowser, C. J. and Dickson, F. W., 1966, Chemical zonation of the borates at Kramer, California, _in_ Rau, J. L., ed., 2nd Symposium on Salt: Northern Ohio Geological Society, Cleveland, Ohio, v. 1, p. 122-132.

Boyd, F. M., 1982, Hydrogeology of the Northern Salt Basin of West Texas and New Mexico: Ph. D. thesis, University of Texas at Austin, p. 61-71.

Braitsch, Otto, 1971, Salt Deposits, their Origin and Composition: Springer-Verlag, 297 p.

Carpenter, A. B., 1978, Origin and chemical evolution of brines in sedimentary basins: Oklahoma Geological Survey Circular 79, p. 60-78.

______, 1979, Interim report on lead and zinc in oil-field brines in the central Gulf Coast and in southern Michigan: AIME Annual Meeting, New Orleans, La., Report 79-95, 15 p.

Clarke, F. E. and Jones, B. F., 1972, Significance of ground-water chemistry in performance of North Sahara tube wells in Algeria and Tunisia: U.S. Geological Survey Water Supply Paper 1757-M, p. 1-39.

Cross, C. W., Iddings, J. P., Pirsson, L. V., and Washington, H. S., 1902, A quantitative chemico-mineralogical classification and nomenclature of igneous rocks: Journal of Geology, v. 10, p. 555-690.

Dickey, P. A., Collins, A. G., and Fajardo, I., 1972, Chemical composition of deep formation waters in southwestern Louisiana: American Association of Petroleum Geologists Bulletin, v. 56, p. 1530-1533.

Drever, J. I., 1982, The Geochemistry of Natural Waters, Prentice Hall, Englewood Cliffs, N. J., 388 p.

Englund, Jens-Olaf, 1983, Chemistry and flow patterns in some ground-waters of southeastern Norway: Norges Geologiske Undersokelse, offprint 380, p. 221-234.

Englund, Jens-Olaf and Myhrstad, J. A., 1980, Groundwater chemistry of some selected areas in southeastern Norway: Nordic Hydrology, v. 11, p. 33-54.

Ericksen, G. E., Chong D., Guillermo, and Vila G., Tomas, 1976, Lithium resources of salars in the central Andes: U.S. Geol. Survey Prof. Paper 1005, p. 66-74.

Eugster, H. P., 1980, Geochemistry of evaporitic lacustrine deposits: Annual Review of Earth and Planetary Science, v. 8, p. 35-63.

Eugster, H. P. and Hardie, L. A., 1978, Saline lakes, _in_ Lerman, A., ed., Lakes: Chemistry, Geology, Physics: Springer-Verlag, New York, p. 237-293.

Eugster, H. P., Harvie, C. E., and Weare, J. H., 1980, Mineral equilibria in the six-component sea water system, Na-K-Mg-Ca-SO_4-Cl-H_2O, at 25°C: Geochimica et Cosmochimica Acta, v. 44, p. 1355-1348.

Eugster, H. P. and Jones, B. F., 1979, Behavior of major solutes during closed-basin brine evolution: American Journal of Science, v. 279, p. 609-631.

Fleischer, E., Goldberg, M., Gat, J. R., and Magaritz, M., 1977, Isotopic composition of formation waters fromm deep drillings in southern Israel: Geochimica et Cosmochimica Acta, v. 41, p. 511-525.

Frape, S. K. and Fritz, Peter, 1982, The chemsitry and isotopic composition of saline groundwaters from the Sudbury Basin, Ontario: Canadian Journal of Earth Sciences, v. 19, p. 645-661.

Frape, S. K., Fritz, Peter, and McNutt, R. H., 1984, Water-rock interaction and chemistry of groundwaters from the Canadian Shield: Geochimica et Cosmochimica Acta, v. 48, p. 1617-1627.

Garrels, R. M., 1967, Genesis of some ground waters from igneous rocks, in Abelson, P. H., ed., Researches in Geochemistry: John Wiley, New York, v. 2, p. 405-421.

Gat, J. R. and Issar, A., 1974, Desert isotope hydrology: water sources of the Sinai Desert: Geochimica et Cosmochimica Acta, v. 38, p. 1117-1131.

Gueddari, Moncef, Monnin, Christophe, Perret, Dominique, Fritz, Bertrand, and Tardy, Yves 1983, Geochemistry of brines of the Cott el Jerid in southern Tunisia -- application of Pitzer's equations: Chemical Geology, v. 39, p. 165-178.

Gulbrandsen, R. A., 1975, Whitlockite and apatite of surficial phosphate occurrences on Enderbury Island, Phoenix Islands, Pacific Ocean: Journal of Research, U. S. Geological Survey, v. 3, p. 409-414.

Hanor, J. S., 1984, Variation in the chemical composition of oil-field brines with depth in northern Louisiana and southern Arkansas: implications for mechanism and rates of mass transport and diagenetic reaction: Transactions--Gulf Coast Association of Geological Societies, v. 34, p. 55-61.

Hardie, L. A. and Eugster, H. P., 1970, The evolution of closed-basin brines: Mineralogical Society of America, Special Publication 3, p. 273-290.

Harvie, C. E., Eugster, H. P., and Weare, J. H., 1982, Mineral equilibria in the six-component seawater system, Na-K-Mg-Ca-SO_4-Cl-H_2O at 25°C. II: Compositions of the saturated solutions: Geochimica et Cosmochimica Acta, v. 46, p. 1603-1618.

Harvie, C. E., Møller-Weare, Nancy, and Weare, J. H., 1984, The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O sytem to high ionic strengths at 25°C: Geochimica et Cosmochimica Acta, v. 48, p. 723-751.

Harvie, C. E. and Weare, J. H., 1980, The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-Cl-SO_4-H_2O system from zero to high concentration at 25°C: Geochimica et Cosmochimica Acta, v. 44, p. 981-997.

Hem, J. D., 1970, Study and interpretation of the chemical characteristics of natural waters: U. S. Geological Survey, Water-Supply Paper 1473, 363 p.

Herrmann, A. G., Knake, Doris, Schneider, Jurgen, and Peters, Heide, 1973, Geochemistry of modern seawater and brines from salt pans: main components and bromine distribution: Contributions to Mineralogy and Petrology, v. 40, p. 1-24.

Holland, H. D., 1984, The Chemical Evolution of the Atmosphere and Oceans: Princeton University Press, Princeton, N. J., 528 p.

Howard, K. W. F. and Lloyd, J. W., 1983, Major ion characterization of coastal saline ground waters: Ground Water, v. 21, p. 429-437.

Jones, B. F., 1966, Geochemical evolution of closed basin water in the western Great Basin, in Rau, J. L., ed., 2nd Symposium on Salt, Northern Ohio Geological Society, Cleveland, Ohio, v. 1, p. 181-200.

______, ed., 1970, Symposium on the mineralogy and geochemistry of non-marine evaporites: Mineralogical Society America, Special Paper 3, p. 213-319.

Knauth, L. P., Kumar, M. B., and Martinez, J. D., 1980, Isotope geochemistry of water in Gulf Coast salt domes: Journal of Geophysical Research, v. 85, p. 4863-4871.

Kühn, Robert, 1968, Geochemistry of the German potash deposits, in Mattox, R. B., ed., Saline Deposits: Geological Society of America Special Paper 88, p. 427-504.

Kumar, M. B., 1983, Character of meteoric leaks in the salt mines of southern Louisiana, USA: Journal of Hydrology, v. 66, p. 351-363.

Lambert, S. J., 1978, Geochemistry of Delaware Basin ground waters: in Austin, G. S., ed., Geology and Mineral Deposits of Ochoan Rocks in Delaware Basin and Adjacent Areas, Mew Mexico Bureau of Mines and Mineral Resources, Circular 159, p. 33-38.

Levy, Yitzhak, 1977, The origin and evolution of brine in coastal sabkhas, northern Sinai: Journal of Sedimentary Petrology, v. 47, p. 451-462.

Livingstone, D. A., 1963, Chemical composition of rivers and lakes, in Fleischer, Michael, ed., Data of Geochemistry [6th ed.]: U.S. Geol. Survey Prof. Paper 440-G, 64 p.

Mackenzie, F. T. and Garrels, R. M., 1966, Chemical mass balance between rivers and oceans: American Journal of Science, v. 264, p. 507-525.

Mann, A. W., 1983,Hydrogeochemistry and weathering on the Yilgarn Block, Western Australia--ferrolysis and heavy metals in continental brines: Geochimica et Cosmochimica Acta, v. 47, p. 181-190.

Marfil, Rafaela, Bermejo, E. P., and de la Pena, J. A., 1975, Sedimentacion salina actual en las lagunas de la zona Corral Rubio-La Higuera (provincia de Albacete): Estudios Geologicos, v. 31, p. 543-553.

Mayhew, E. J. and Heylmun, E. B., 1965, Concentrated subsurface brines in the Moab Region, Utah: Utah Geological and Mineralogical Survey, Special Studies 13, 28 p.

Muessig, Siegfried, 1958, First known occurrence of inyoite in a playa, at Laguna Salinas, Peru: American Mineralogist, v. 43, p. 1144-1147.

_____, 1959, Primary borates in playa deposits: Minerals of high hydration: Economic Geology, v. 54, p. 495-501.

_____, 1966, Recent South American borate deposits, in Rau, J. L., ed., 2nd Symposium on Salt: Northern Ohio Geological Society, Cleveland, Ohio, v. 1, p. 151-159.

Parker, V. B., Wagman, D. D., and Evans, W. H., 1971, Selected values of chemical thermodynamic properties: Tables for the alkaline earth elements, National Bureau of Standards: Technical Note 270-6, 106 p.

Plummer, L. N., Jones, B. F., and Truesdell, A. H., 1976, WATEQF - a Fortran IV version of WATEQ, a computer program for calculating chemical equilibrium of natural waters: U.S. Geological Survey Water-Resources Investigations 76-13, 61 p.

Rankama, Kalervo and Sahama, Th. G., 1950, Geochemistry: University of Chicago Press, 912 p.

Riley, J. P. and Chester, R., 1971, Introduction to Marine Chemistry: Academic Press, New York, 465 p.

Rettig, S. L., Jones, B. F., and Risacher, Francois, 1980, Geochemical evolution of brines in the Salar of Uyuni, Bolivia: Chemical Geology, v. 30, p. 57-79.

Robie, R. A., Hemingway, B. S., and Fisher, J. R., 1978, Thermodynamic properties of minerals and related substances at 298.15 K and 1 bar (10^5 pascals) pressure and at higher temperatures: U.S. Geological Survey Bulletin 1452, 456 p.

Smith, G. I. and Haines, D. V., 1964, Character and distribution of nonclastic minerals in the Searles Lake evaporite deposit, California: U.S. Geological Survey Bulletin 1181-P, 58 p.

Sonnenfeld, Peter, 1984, Brines and Evaporites: Academic Press, New York, 613 p.

Soriano, Jose, Marfil, Rafaela, and de la Pena, J. A., 1977, Sedimentacion salina actual en las lagunas del norte de Alcazar de San Juan (Ciudad Real): Estudios Geologicos, v. 33, p. 123-130.

Spencer, R. J., Eugster, H. P., Jones, B. F., and Rettig, S. L., 1983, Geochemistry of Great Salt Lake, Utah I: Hydrochemistry since 1850:: Geochimica et Cosmochimica Acta, v. 49, p. 727-737.

Starinsky, A., Bielski, M., Ecker, A., and Steinitz, G., 1983, Tracing the origin of salts in groundwater by Sr isotopic composition (the crystalline complex of the Southern Sinai, Egypt): Isotope Geoscience, v. 1, p. 257-267.

Stewart, D. B., Jones, B. F., Roedder, E. W., and Potter, R. W., 1980, Summary of United States Geological Survey Investigations of fluid-rock-waste reactions in evaporite environments under repository conditions from "Underground Disposal of Radioactive Waste,": International Atomic Energy Agency, Vienna, 1980, v. 1, p. 335-344.

Stewart, F. J., 1963, Marine evaporites, in Fleischer, Michael, ed., Data of Geochemistry (6th ed.): U. S. Geological Survey Professional Paper 440-Y, 53 p.

Stoessel, R. K., and Moore, C. H., 1983, Chemical constraints and origins of four suggested groups of Gulf Coast Reservoir fluids: American Association of Petroleum Geologists Bulletin, v. 67, p. 896-906.

Truesdell, A. H. and Jones, B. F., 1974, WATEQ: A computer program for calculating chemical equilibria of natural waters: U.S. Geological Survey, Journal of Research, v. 2, p. 233-248.

Wagman, D. D., Evans, W. H., Parker, V. B., Halow, I., Bailey, S. M., and Schumm, R. H., 1968, Selected values of chemical thermodynamic properties: Tables for the first thirty-four elements in the standard order of arrangement: National Bureau of Standards, Technical Note 270-3, 264 p.

Wagman, D. D., Evans, W. H., Parker, V. B., Schumm, R. H., and Nuttall, R. L., 1981, Selected values of chemical thermodynamic properties: Compounds of uranium, protactinium, thorium, actinium, and the alkali metals: National Bureau of Standards, Technical Note 270-8, 134 p.

Wedepohl, K. H., 1971, Geochemistry: Holt, Renehart, and Winston, New York, 231 p.

White, D. E., 1968, Environments of generation of some base-metal ore deposits: Economic Geology, v. 63, p. 301-335.

White, D. E., Hem, J. D., and Waring, G. A., 1963, Chemical composition of subsurface waters, _in_ Fleischer, Michael, ed., Data of Geochemistry [6th ed.]: U.S. Geol. Survey Prof. Paper 440-F, 67 p.

Zak, Israel and Gat, J. R., 1975, Saline waters and residual brines in the Shiraz-Sarvistan Basin, Iran: Chemical Geology, v. 16, p. 179-188.

Zherebtsova, I. K. and Volkova, N. N., 1966, Experimental study of behavior of trace elements in the process of natural solar evaporiation of Black Sea water and Sasyk-Sivash brine: Geochemistry International, v. 3, p. 656-670.

APPENDIX I

Source codes

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c***********************************************************************
c                                 SNORM
c***********************************************************************
c                                                             April 1986
c
c     Bodine, M. W., Jr. and Jones, B. F. (in press), The salt norm:  a
c       quantitative chemical-mineralogical characterization of natural
c       waters:  U.S. Geological Survey, Water-Resources Investigations
c       Report 86-4086.
c
c   SNORM reads concentration data for inorganic solutes in natural wa-
c   ters, proportions cation and anion concentrations to yield charge
c   balance, and combines the adjusted constituent solutes into an equi-
c   librium crystalline salt assemblage or "salt norm."  This salt norm
c   can be considered as the equilibrium assemblage of salts persisting
c   with evaporation to dryness (all free water removed) at 25 degrees
c   Celsius and one atmosphere pressure.  A related "simple salt assem-
c   blage," derived from the salt norm, is also calculated.
c
c   The program accepts concentrations for eighteen solutes that common-
c   ly occur as major or minor constituents in standard water analyses.
c   Solutes which are rarely observed in more than trace quantities are
c   not considered in calculating normative assemblages.  In addition,
c   manganese, iron, reduced sulfur species, and reduced carbon species
c   are not considered because of redox difficulties, and, because of
c   silicon-oxygen polymerization in crystalline silicates, dissolved
c   silica is not considered.
c
c   SNORM provides the following:
c
c     1. Either retrieval from the user's directory of a previously en-
c        tered input file of a group of water descriptions and analyses,
c        or creation and storage of a new input file.  The input file
c        may be written or read by SNORM in the format established for
c        SNORM, or in the more comprehensive WATEQ format (Plummer,
c        Jones, and Truesdell, 1976, U.S. Geol. Survey, Water Resources
c        Investigations 76-13).  This allows use of input data files in
c        the WATEQ format to be written and read by both SNORM and
c        WATEQ or WATEQF.
c
c        If retrieval of an existing file is elected, the user enters
c        file name (a10) when requested; requests a listing of samples
c        in the file, if desired; and, if desired, identifies specific
c        sample(s) for computation.  Program proceeds to step 3 below.
c
c     2. Creation of a new input data file.  The user names the proposed
c        file (a10), and specifies either the WATEQ or SNORM format for
c        the file.  User may also designate that only the new file be
c        created by SNORM, thus omitting any salt norm calculations and
c        output.
c
c        If the user anticipates evaluating the analyses for the extent
c        of salt saturation and defining the thermodynamic properties of
c        the water sample, an input file in the WATEQ format is recom-
c        mended.  See Plummer, Jones, and Truesdell (1976), cited previ-
c        ously, for entering a WATEQ input file.
c
c        The SNORM format involves less extensive entry per sample and
c        is recommended if either the analysis is incomplete (lacks one
c        or more of pH, temperature, redox data or Eh, alkalinity), or
c        the results from WATEQ are unwanted.
c
c        The SNORM input file format consists of a first line (a80)
c        that is the title for the group of analyses to be entered in
c        the file.  This is followed by a sequence of 3-to-5 lines for
c        each sample in the group.
c
c           Line 1: a. Sample number (a10).
c                   b. Sample pH (f5); 20.0 if unknown.
c                   c. Sample density (f5); 0.0 if unknown.
c                   d. Solute analytical units (i1) as a single digit
c                      identifier integer code (1 - molality, 2 - mg/kg,
c                      3 - meq/liter, 4 - mg/liter, 5 - moles/liter); no
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c                     entry or an entry of 0 for the analytical-unit-
c                     identifier integer signifies that the previous
c                     analysis is to be the last analysis in the file.
c                  e. Brief sample description (a40).
c
c          Line 2: Concentrations of six major solutes (Ca, Mg, K, Na,
c             Cl, SO4) in analytical units specified above (5e11).
c
c          Line 3: Concentrations of other solutes in analytical units
c             specified above; a solute identifier (i2) and its concen
c             tration (e10) is entered for up to 5 solutes per line; if
c             a line becomes filled with solute data, a new line be
c             comes available; no entry or entering 00 for the solute-
c             identifier integer after all permissable solutes have
c             been entered signifies conclusion of entry for that sam-
c             ple, and, after verification, line 1 returns to allow en-
c             tering data for the next sample in the group.
c
c       After each line is entered during construction of an input file
c       (in either WATEQ or SNORM format), the line is printed at the
c       user's terminal and verification is requested.  If entry is
c       correct, the entry is verified and the line is appended onto
c       the developing input file; if not verified, the user is reques-
c       ted to reenter the line.
c
c       After completing entry into the new input file, the file is
c       stored in the user's directory under the assigned name.
c
c    3. User selection of the following options for all samples in a
c       given input file:
c
c       a. Output of SNORM data bank.  User may designate output of
c          the data bank that lists all solutes, each with its charge
c          and atomic weight, and all salts, each with its mineral
c          name, chemical formula, and composition in terms of the sol-
c          ute species.  Additional species (O, OH, and H2O) are in
c          cluded with the solutes to facilitate calculating salt com-
c          positions and molecular weights.
c
c       b. Capability of the output device.  User designates if output
c          to be directly displayed or printed, and, if so, whether the
c          output device accepts line length of <132 characters (output
c          formatted at 80 characters per line) or >131 characters
c          (output formatted at 132 characters per line).
c
c       c. Storage of output.  User may request creation of SNORM out
c          put file(s), formatted at 132 characters per line, that will
c          be stored in the user's directory for subsequent printing.
c          User designates if the requested output file(s) will be con-
c          structed to be read by printer that recognizes FORTRAN car-
c          riage control, one that does not, or both.
c
c       d. Alternative concentration units of solutes and normative
c          salts.  Concentrations of the normative salts for each sam-
c          ple are listed in weight and moles per unit of the original
c          analysis, i.e. "per kg water," "per kg solution," or "per
c          liter solution."  The user may designate salt concentrations
c          be listed in units other than those of the analysis, and if
c          so elected, solute concentrations will be listed in both the
c          requested units and the units of the analysis, and normative
c          salt concentrations will be listed in the requested units.
c          If recasting between "per kg" and "per liter" units is pre-
c          scribed, density of the sample must be known; if density un-
c          known, original units of the analysis will be retained.
c
c       e. Listing of salt equivalencies rather than mole abundances.
c          User may designate that normative salt abundances be listed
c          in salt equivalencies (concentration and percent) rather
c          than in mole quantities.  A salt equivalent is defined as
c          the product of the anion charge of a mole of the salt and
c          the salt's mole abundance.
c
c       f. Redox reassignment of nitrogen species.  User may specify
c          redox state of nitrogen species (ammonium and nitrate) be
c          assigned so that either any ammonium is recast as nitrate,
c          or, alternatively, any nitrate is recast as ammonium.
c
c       g. Reassignment of nitrate as bicarbonate.  If the user wishes
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c           to eliminate nitrate from the norm without affecting the
c           original solute charge distribution, he may elect to substi-
c           tute bicarbonate for nitrate.  Had the user elected to con-
c           vert ammonium to nitrate, this nitrate would also be trans-
c           formed to bicarbonate.
c
c        h. Assignment of zero concentration to one or more solutes.
c           User may elect to determine the norm excluding one or more
c           solutes from the calculation; this is accomplished by iden-
c           tifying from 1 to 10 solutes whose concentrations are to be
c           set to 0.0 prior to adjusting for charge balance.
c
c        Election of one or more options from (f) through (h) above may
c        affect the salt norm by altering solute characteristics of the
c        sample.  Election of these options does not alter the output
c        listing of solute concentrations in the original analysis; the
c        results of the elected options are included and identified in
c        the output listing of solute concentrations that are adjused to
c        achieve charge balance.
c
c        These options, (f) through (h), are only available to the user
c        if a previously stored input file is retrieved by SNORM; they
c        are not available if a new input file is created.  The norm for
c        any sample in the input file whose adjusted solute concentra-
c        tions (and the resultant salt norm) are not altered after im-
c        plementing the elected option(s) is not calculated, and all
c        output for that sample is omitted.
c
c        Each option (a through h) is entered as a response to a query
c        with a listing of the alternative responses displayed on the
c        user's terminal; the user enters the appropriate response fol-
c        lowed by a <RETURN>.
c
c     4. Calculation and printing of the following for each sample in
c        the file: (a) solute concentrations in weight and mole quanti
c        ties for both the analytical values of the original analysis
c        and the modified values that have been adjusted to achieve
c        charge balance; (b) mole ratios from the original analytical
c        data; (c) the normative salt assemblage with weight (both for
c        correct hydration state of the salt and for its anhydrous equi-
c        valent) and mole concentrations of each normative salt per unit
c        of solution, and weight (again for correct hydration state and
c        its anhydrous equivalent) and mole percentages in the solid as
c        semblage; (d) a simple salt assemblage that is derived from the
c        normative assemblage with weight and mole percent of each sim-
c        ple salt in the simple salt assemblage; and (e) a summary of
c        calculations required to calculate the norm (number of salt as
c        sociations tested, number of trial assemblages created, and
c        number of trial assemblages for which salt abundances were de-
c        termined).  A title for the group of samples in the file, sam-
c        ple description (sample number, location, brief description),
c        other analytical data (pH, density), footnotes identifying
c        elected options, and the date of calling SNORM are also
c        printed for each sample; and, if requested, the SNORM data
c        bank is listed at the beginning of the output.
c
c   Solutes, normative salts, and simple salts
c   ------------------------------------------
c
c   Solutes that are assigned to the normative salt assemblage comprise
c   the following.
c
c              Mg++    Ba++    K+      HCO3-   Cl-     F-
c              Ca++    Li+     NH4+    CO3--   Br-     NO3-
c              Sr++    Na+     B       SO4--   I-      PO4---
c
c   Carbonate and bicarbonate are mutually interchangeable throughout
c   calculation of normative salt and simple salt assemblages through
c   the reaction, 2HCO3- = CO3-- + H2O + CO2, which conserves total bi-
c   carbonate-carbonate charge.  Bromide and iodide are assigned propor-
c   tionately to chloride salts as solid solution components.  Elemental
c   boron of the analysis is assigned to normative salts as the appro-
c   priate borate polymer; the adjustment to achieve solute charge bal-
c   ance includes the negative charge of the borate polymer.
c
c   The solutes are combined to form the salt norm from the following
c   list of permissable normative salts.
c
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c     BICARBONATES/CARBONATES
c       Calcite         Trona           Strontionite    Teschemacherite
c       Dolomite        Pirssonite      Witherite       Li2CO3
c       Magnesite       Kalicinite
c     SULFATES
c       Anhydrite       Mirabilite      Bloedite        Celestite
c       Gypsum          Arcanite        Leonite         Barite
c       Kieserite       Glauberite      Picromerite     Mascagnite
c       Epsomite        Syngenite       Aphthitalite    Li2SO4.H2O
c       Thenardite      Polyhalite      Burkeite        Kainite
c     CHLORIDES (including bromide and iodide)
c       Antarcticite    Carnallite      SrCl2.2H2O      BaCl2.2H2O
c       Tachyhydrite    Sylvite         SrCl2.6H2O      Salammoniac
c       Bischofite      Halite          BaCl2.H2O       LiCl.H2O
c     NITRATES
c       Nitrocalcite    Niter           Sr(NO3)2        Ammonia niter
c       Nitromagnesite  Soda niter      Nitrobarite     LiNO3.3H2O
c     BORATES
c       Inyoite         Indirite        Borax           Ulexite
c     FLUORIDES
c       Fluorite        Sellaite        Villiaumite     LiF
c     PHOSPHATES
c       Hydroxyapatite  Mg3(PO4)2       Wagnerite       Na3PO4
c       Fluorapatite
c
c   Several of the above salts are double anion salts; burkeite is a
c   sulfate-carbonate, kainite is a sulfate-chloride, fluorapatite and
c   wagnerite are phosphate-fluorides, and hydroxyapatite is a phos-
c   phate-hydroxide.  Since hydroxide is not a solute that is included
c   in the adjustment to achieve charge balance, normative hydroxyapa-
c   tite is calculated as Ca4.75(PO4)3.17.
c
c   In normative assemblages that contain two of more coexisting borate
c   salts, other than the inyoite-indirite pair, the differing boron-
c   oxygen polymers in the coexisting borates require forming an inter-
c   mediate borate polymer and redefining the borate salt compositions
c   as borax - Na(2.28)B(3.91)O7, indirite - Mg(1.79)B(6.14)O11, ulexite
c   - Na(0.98)Ca(0.98)B(5.02)O9, and inyoite - Ca(1.79)B(6.14)O11 with
c   each having their proper number of hydration waters.
c
c   Normative salts that are composed of major solute cations (Ca, Mg,
c   K, and Na) and anions (HCO3/CO3, SO4, and CL) are recast into the
c   following simple salts.
c
c              CaCO3   K2CO3   CaSO4   K2SO4   CaCl2   K2Cl2
c              MgCO3   Na2CO3  MgSO4   Na2SO4  MgCl2   Na2Cl2
c
c   The simple carbonate salts are produced from any normative bicarbon-
c   ate salts without altering total carbonate-bicarbonate charge
c   through the reaction given above.  The alkali chloride simple salts
c   are assigned stoichiometries of Na2Cl2 and K2Cl2 so that cation
c   charge of each simple salt is 2+.
c***********************************************************************
      character*80 jbatch
      character*40 kdes
      character*10 knum
      dimension kdes(99),knum(99),kx(3,99),jbatch(99),kud(99)
      character*80 nbatch
      character*40 ndes
      character*20 mf
      character*15 nmin
      character*13 nsimp,lout,lloc
      character*10 nfile,nnum
      character*5 ncom
      common ncom(25),atw(25),nv(25),v(25),va(25),chg,kbor,nitro,np,kid,
     a ncfn,nnox,nc,cz(25,14),nnax,lout,kbri,kfile,s(99),kred,npage,kxt,
     c isalt(99),lunit,konf,nix(25),nnix,x(25),xo(25),c(25),lloc,nbatch,
     d kend,to(25),kid2,kfirst,kpage,ndes,nnum,nuts,nmin(99),kbank,kidl,
     e nfile,muts,mf(99),lc(99,6),lz(99,6),lh(99),la(99),z(99,6),ph,den,
     f must(10),nsimp,nu(10),naly(99),kid3,mp(9),mr(9),ctz(14),nax(25)
      kod = 0
      mp(4) = 1
      mp(5) = 0
      if(mp(4).ne.0) go to 11
      do 10, i=1,10
      nu(i) = 20 + i
      if(i.eq.10) nu(i) = 0
   10 continue
```

```
 11 continue
    if(mp(4).ne.1) go to 21
    do 20 i=1,10
    nu(i) = 10 + i
    if(i.eq.4) nu(i) = 5
    if(i.eq.9) nu(i) = 14
    if(i.eq.10) nu(i) = 1
 20 continue
 21 continue
    call prep
    if(kpage.eq.3) go to 900
    konf = 0
    open(nu(2),form='formatted',status='old',file=nfile,err=100)
    if(kfile.eq.0) go to 200
    if(kfile.ne.2) open(nu(4),form='formatted',status='new',file=lout)
    if(kfile.ne.1) open(nu(5),form='formatted',status='new',file=lloc)
    go to 200
100 continue
    go to 800
200 continue
    kidl = 0
    kfirst = 0
300 continue
    call load
    kidl = kidl + 1
    if(kid3.eq.1) print 810
    if(kend.eq.1) go to 500
    if(nnox.eq.0) go to 450
    call join
    kod = kod + 1
    kud(kod) = kidl
    if(kid.eq.0) kdes(kod) = ndes
    if(kid.eq.0) knum(kod) = nnum
    if(kid.eq.1) jbatch(kod) = nbatch
    do 400  i=1,3
    kx(i,kod) = mr(i)
400 continue
450 continue
    go to 300
500 continue
    if(kidl.eq.0) go to 800
    if(kod.eq.0) go to 800
    if(kpage.lt.2) lunit = nu(10)
    if(kpage.eq.2.and.kfile.ne.2) lunit = nu(4)
    if(kpage.eq.2.and.kfile.eq.2) lunit = nu(5)
600 continue
    write(lunit,801)
    if(kid.eq.0) write(lunit,805) nbatch
    do 700 i=1,kod
    if(kid.eq.0) write(lunit,802) kud(i),knum(i),kdes(i)
    if(kid.eq.1) write(lunit,804) kud(i),jbatch(i)
    write(lunit,803) (kx(j,i),j=1,3)
700 continue
    if(kfile.eq.0.or.lunit.eq.nu(5)) go to 800
    if(lunit.eq.nu(4).and.kfile.eq.1) go to 800
    if(lunit.eq.nu(4)) lunit = nu(5)
    if(lunit.lt.nu(4).and.kfile.ne.2) lunit = nu(4)
    if(lunit.lt.nu(4)) lunit = nu(5)
    go to 600
800 continue
    close(nu(2))
    if(mp(5).eq.1) close(nu(7))
    if(kfile.eq.0) go to 900
    if(kfile.ne.2) close(nu(4))
    if(kfile.ne.1) close(nu(5))
900 continue
    stop
801 format('1',////,19x,'SUMMARY OF REQUIRED CALCULATIONS',/)
802 format(' ',i2,'. ',a10,15x,a40)
803 format(' ',3x,'Salt-pair tests =',i6,7x,'Assemblage tests =',
   a i4,7x,'Inversions =',i4,/)
805 format(' ',/,a80,/)
804 format(' ',i2,'. ',a80)
810 format(' ','Unable to read input file in either SNORM or',
   a' WATEQ format!!',/20x,'RUN TERMINATED')
    end
c***********************************************************************
```

```
c***********************************************************************
c                          Subroutine PREP
c***********************************************************************
c
c   Reading file of data constants (NEODAT) for solutes and salts;
c   accepting identity of input data file; accepting user-specified
c   output format and concentration units; and accepting input data if
c   SNORM format elected.
c
      subroutine prep
      character*2 jyy,jzz,jyz
      character*3 jjy,jjz,jzy
      character*8 neld,meld
      character*13 nart,llot
      character*80 kbatch,kempty
      dimension cc(5),ic(5),iic(5),nox(10),neld(2),nuse(25),jjy(5),
     a jjz(5)
      character*80 nbatch
      character*40 ndes
      character*20 mf
      character*15 nmin
      character*13 nsimp,lout,lloc
      character*10 nfile,nnum
      character*5 ncom
      common ncom(25),atw(25),nv(25),v(25),va(25),chg,kbor,nitro,np,kid,
     a ncfn,nnox,nc,cz(25,14),nnax,lout,kbri,kfile,s(99),kred,npage,kxt,
     c isalt(99),lunit,konf,nix(25),nnix,x(25),xo(25),c(25),lloc,nbatch,
     d kend,to(25),kid2,kfirst,kpage,ndes,nnum,nuts,nmin(99),kbank,kidl,
     e nfile,muts,mf(99),lc(99,6),lz(99,6),lh(99),la(99),z(99,6),ph,den,
     f must(10),nsimp,nu(10),naly(99),kid3,mp(9),mr(9),ctz(14),nax(25)
      data jyy/'p.'/
      data jzz/'t.'/
      data jjy/'p2.','p3.','p4.','p5.','p6.'/
      data jjz/'t2.','t3.','t4.','t5.','t6.'/
      data neld/'existing','proposed'/
  100 continue
      kfile = 0
      konf = 0
      kid = 0
      npage = 0
      mp(9) = 0
c
c                  Defining source of and naming input data file
c
      print 805
      read 801,konf
      if(konf.eq.0) meld = neld(1)
      if(konf.ne.0) meld = neld(2)
  105 continue
      print 810,meld
      read 800,nfile
      open(nu(9),form='formatted',status='old',file=nfile,err=110)
      read(nu(9),910,end=110,err=110) nbatch
      close(nu(9))
      if(konf.eq.0) go to 125
      print 824,nfile
      read 801,i
      if(i-1)105,115,109
  109 continue
      if(i.eq.3) kpage = 3
      if(i.eq.3) go to 995
      konf = 0
      go to 125
  110 continue
      close(nu(9))
      if(konf.eq.1) go to 115
      print 815,nfile
      read 801,i
      if(i.eq.0) go to 100
      kpage = 3
      go to 995
  115 continue
      print 825
      read 801,kid
  125 continue
c
c       Listing file and selecting specific-samples option
c
```

```
      nsel = 0
      if(konf.eq.1) go to 147
      print 811
      read 801,i
      if(i.eq.0) go to 139
      kadl = 0
      nolist = 0
      open(nu(6),form='formatted',status='old',file=nfile,err=126)
      go to 127
  126 continue
      nolist = 1
      print 816
      go to 138
  127 continue
      read(nu(6),910) nbatch
  128 continue
      read(nu(6),930,err=131,end=138) nnum,ndes,ph,den,nuts
      if(kadl.eq.0.and.nuts.eq.0) go to 131
      if(nuts.eq.0) go to 138
      kadl = kadl + 1
      if(kadl.eq.1) print 910, nbatch
      if(kadl.eq.1) print 854
      print 813, kadl,nnum,ndes
      read(nu(6),940,err=126,end=138)(c(i),i=1,6)
  129 continue
      read(nu(6),960,err=126,end=138)(ic(i),cc(i),i=1,5)
      do 130 i=1,5
      if(ic(i).eq.0) go to 128
  130 continue
      go to 129
  131 continue
      rewind nu(6)
      kadl = 0
      write(kbatch,818)
      read(kbatch,910) kempty
      print 854
  132 continue
      read(nu(6),910,end=138) kbatch
      kadl = kadl + 1
      print 814,kadl,kbatch
      read(nu(6),910,err=126,end=138) kbatch
      read(nu(6),910,err=126,end=138) kbatch
      read(nu(6),910,err=126,end=138) kbatch
      do 133 j=1,20
      read(nu(6),910,err=126,end=138) kbatch
      if(kbatch.eq.kempty) go to 132
  133 continue
  138 continue
      close(nu(6))
  139 continue
      print 821
      read 801,nsel
      if(nsel.eq.0) go to 147
      if(nsel.eq.2) go to 146
  140 continue
      print 822
      read(nu(10),823,err=142)(nuse(k),k=1,25)
      go to 144
  142 continue
      print 803
      go to 140
  144 continue
      print 823,(nuse(k),k=1,25)
      print 802
      read 801,nerr
      if(nerr.ne.0) go to 140
      if(nsel.eq.1) go to 147
  146 continue
      if(nsel.eq.2) nsel = 0
      mp(9) = 1
  145 continue
      print 847
      read(nu(10),870,err=1451)(must(i),i=1,10)
      go to 1452
 1451 continue
      print 803
      go to 145
 1452 continue
```

```
      print 870,(must(i),i=1,10)
      print 802
      read 801,nerr
      if(nerr.ne.0) go to 145
  147 continue
      do 150 i=1,99
      naly(i) = 0
      if(konf.eq.1.or.nsel.eq.0) naly(i) = 1
      if(naly(i).eq.1) go to 150
      do 148 k=1,25
      if(nuse(k).eq.i) naly(i) = 1
  148 continue
  150 continue
c
c     Loading data bank for dissolved components and salt phases
c
      open(nu(3),form='formatted',status='old',file='neodat')
      do 155 i=1,25
      read(nu(3),890) ncom(i),atw(i),nv(i)
      if(atw(i).eq.0.0) go to 160
      nc = i
      v(i) = float(nv(i))
      va(i) = abs(v(i))
  155 continue
  160 continue
      mr(7) = 0
      np = 0
      jj = 0
      do 175    j=1,99
      i = j - jj
      read(nu(3),895,end=180) nmin(i),mf(i),(lc(i,k),lz(i,k),k=1,6)
      if(lc(i,1).eq.0) go to 170
      do 165    k=1,6
      if(lc(i,k).eq.0) go to 175
      lh(i) =  k
      z(i,k) =  float(lz(i,k))
      if(lc(i,k).eq.19) go to 165
      la(i) = k
  165 continue
      go to 175
  170 continue
      if(np.gt.0) go to 180
      np = j - 1
      mr(7) = j
      jj = 1
  175 continue
  180 continue
      mr(8) = j - 2
      v(14) = -7.0/12.0
      va(14) = abs(v(14))
      close(nu(3))
c
c               Selecting output destination and format
c
      print 830
      if(konf.eq.1) print 831
      read 801,kpage
      if(kpage.ne.3) go to 205
      konf = 1
      go to 600
  205 continue
      print 835
      if(kpage.lt.2) print 836
      print 837
      read 801,kfile
      if(kfile.eq.0) go to 290
      print 854
      nn = 0
  210 continue
      nn = nn + 1
      if(kfile.eq.2) nn = nn + 1
      if(nn.eq.1) jyz = jyy
      if(nn.gt.1) jyz = jzz
      do 250 i=1,6
      ii = i - 1
      if(ii.ne.0) go to 230
      write(nart,845) jyz,nfile
      read(nart,850) llot
```

```
      go to 240
  230 continue
      if(nn.eq.1) jzy = jjy(ii)
      if(nn.gt.1) jzy = jjz(ii)
      write(nart,848) jzy,nfile
      read(nart,851) llot
  240 continue
      open(nu(4),form='formatted',status='old',file=llot,err=260)
      read(nu(4),910,err=260,end=260) kbatch
      close(nu(4))
  250 continue
      print 961
      kpage = 3
      go to 995
  260 continue
      if(nn.eq.1) lout = llot
      if(nn.gt.1) lloc = llot
      close(nu(4))
      if(nn.eq.1) print 855,lout
      if(nn.gt.1) print 860,lloc
      if(nn.eq.1.and.kfile.ne.1) go to 210
  290 continue
      print 854
c
c                    Electing calculation options
c
  300 continue
      kbank = 0
      kred = 0
      nitro = 0
      ncfn = 0
      nnix = 0
      mr(9) = 0
      do 310 i=1,25
      nix(i) = 0
      if(i.lt.11) nox(i) = 0
  310 continue
  315 continue
      print 861
      if(konf.eq.0) print 862
  320 continue
      read 801,ipt
      if(ipt.eq.0) go to 375
      if(ipt.eq.1) kbank = 1
      if(ipt.eq.2) go to 360
      if(ipt.eq.3) mr(9) = 1
      if(ipt.eq.4) nitro = 1
      if(ipt.eq.5) nitro = 2
      if(ipt.eq.6) ncfn = 1
      if(ipt.eq.7) go to 330
      if(ipt.eq.1) print 881
      if(ipt.eq.3) print 886
      if(ipt.eq.4) print 883
      if(ipt.eq.5) print 884
      if(ipt.eq.6) print 885
  325 continue
      print 880
      go to 320
  330 continue
      print 865
      read(nu(10),870,err=335)(nox(i),i=1,10)
      go to 340
  335 continue
      print 803
      go to 330
  340 continue
      do 345 i=1,10
      if(nox(i).eq.0) go to 350
      nnix = 1
      nix(nox(i)) = 1
      print 875,ncom(nox(i))
  345 continue
  350 continue
      nnix = 0
      if(nitro.eq.1.or.ncfn.ne.0) nix(11) = 0
      if(nitro.eq.2) nix(10) = 0
      do 355 i=1,nc
      if(nix(i).ne.0.0) nnix = 1
```

```
  355 continue
      go to 315
  360 continue
      print 863
      read 801,kred
      if(kred.eq.1) print 896
      if(kred.eq.2) print 897
      if(kred.eq.3) print 898
      go to 325
  375 continue
      sum = kbank+kred+nitro+ncfn+nnix+mr(9)
      if(sum.gt.0) print 888
      if(sum.eq.0) print 889
      if(sum.eq.0) go to 390
      if(kbank.eq.1) print 881
      if(kred.eq.1) print 896
      if(kred.eq.2) print 897
      if(kred.eq.3) print 898
      if(mr(9).eq.1) print 886
      if(nitro.eq.1) print 883
      if(nitro.eq.2) print 884
      if(ncfn.eq.1) print 885
      if(nnix.eq.0) go to 390
      do 385 i=1,nc
      if(nix(i).ne.0) print 875,ncom(i)
  385 continue
  390 continue
      print 854
      print 804
      read 801,i
      if(i.ne.0) go to 300
      write(nsimp,899) nfile
      open(nu(7),file=nsimp,status='new',err=405)
      mp(5)=1
      go to 410
  405 continue
      close(nu(7))
  410 continue
c
c                        Creating new file -- SNORM format
c
  600 continue
      if (konf.eq.0) go to 990
      open(nu(1),form='formatted',status='new',file=nfile)
      if(kid.eq.1) go to 700
  605 continue
      print 905
      read 910,nbatch
      print 910,nbatch
      print 802
      read 801, nerr
      if(nerr.eq.1) go to 605
      write(nu(1),910) nbatch
      n = 0
c                                             Sample number and description
  610 continue
      n = n + 1
      if(n.lt.100) go to 615
      write(nu(1),854)
      print 919
      go to 695
  615 continue
      print 920,n
      read(nu(10),925,err=620)nnum,ph,den,nuts,ndes
      go to 625
  620 continue
      print 803
      go to 615
  625 continue
      print 925,nnum,ph,den,nuts,ndes
      print 802
      read 801, nerr
      if(nerr.eq.1) go to 615
      write(nu(1),930) nnum,ndes,ph,den,nuts
      if(nuts.eq.0) go to 695
c                                                      Major component data
  630 continue
      do 635 i=1,nc
```

```
      c(i) = 0.0
  635 continue
      print 935,n
      read(nu(10),940,err=640)(c(i),i=1,6)
      go to 645
  640 continue
      print 803
      go to 630
  645 continue
      print 940,(c(i),i=1,6)
      print 802
      read 801, nerr
      if(nerr.eq.1) go to 630
      write(nu(1),940) (c(i),i=1,6)
c                                                Other component data
      print 945,n
  650 continue
      do 655   i=1,5
      iic(i) = 0
      ic(i) = 0
      cc(i) = 0.0
  655 continue
      print 950
      read(nu(10),955,err=660)(ic(i),cc(i),i=1,5)
      go to 670
  660 continue
      print 803
      go to 650
  670 continue
      print 955,(ic(i),cc(i),i=1,5)
      print 802
      read 801, nerr
      if(nerr.eq.1) go to 650
      do 675   i=1,5
      if(ic(i).eq.0) go to 680
      if(ic(i).eq.1) iic(i) =  8
      if(ic(i).eq.2) iic(i) = 17
      if(ic(i).eq.3) iic(i) =  9
      if(ic(i).eq.4) iic(i) = 10
      if(ic(i).eq.5) iic(i) = 11
      if(ic(i).eq.6) iic(i) = 12
      if(ic(i).eq.7) iic(i) = 13
      if(ic(i).eq.8) iic(i) = 14
      if(ic(i).eq.9) iic(i) = 18
      if(ic(i).eq.10) iic(i) = 19
      if(ic(i).eq.11) iic(i) = 20
      if(ic(i).eq.12) iic(i) = 21
  675 continue
  680 continue
      write(nu(1),960) (iic(i),cc(i),i=1,5)
      do 685 i=1,5
      if(ic(i).eq.0) go to 690
  685 continue
      go to 650
  690 continue
      go to 610
  695 continue
      go to 900
  700 continue
      call salwat
  900 continue
      close(nu(1))
  990 continue
      if(kpage.eq.3) go to 995
      if(kpage.eq.0) print 975
      if(konf.eq.0) print 980
      if(konf.ne.0) print 985,nfile
      read 801,iiii
      if(iiii.eq.9) go to 100
      if(iiii.eq.8) kpage = 3
  995 continue
      konf = 0
      return
  800 format(a10)
  801 format(i1)
  802 format(' ','Is this entry correct ("0" = yes; "1" = no)??')
  803 format(' ','INPUT ERROR -- re-enter these data!')
  804 format(' ','Acceptable??  "0"=yes; "1"=no')
```

```
805 format(' ',10x,'INPUT DATA SOURCE, OUTPUT OPTIONS, AND ',
   a'NEW INPUT DATA ENTRY',/,
   a18x,'(After each line of entry -- enter <RETURN>)',//,1x,
   a'Status of water analyses for salt norm calculation',
   a' (ENTER one code integer):',/,3x,
   b'"0"  Analyses currently on file as segment in',
   c' user''s directory',/3x,'"1"  Analyses to be entered',
   d' and form a new data segment')
810 format(' ','ENTER NAME of ',a8,' input data segment',
   a ' (up to 10 character string):')
811 format(' ','Listing of samples in file??  "0" = no; "1" = yes')
813 format(i2,'.',5x,a10,10x,a40)
814 format(' ','Sample ',i2,/,a80)
816 format(' ','SORRY -- Unable to list samples!')
818 format(10('        '))
821 format(' ','Selection of samples in file for output:',/,5x,
   a'"0" All samples in file.',/,5x,
   b'"1" Only those to be listed by position in file.',/,5x,
   c'"2" Only those with solutes to be specified.',/,5x,
   d'"3" Both "1" and "2" above.')
822 format(' ','Enter up to 25 two-integer identifiers:',/,
   1 24('--',1x),'--')
823 format(24(i2,1x),i2)
919 format(' ',16x,'99 analyses entered in file -- file full!',/,
   1 28x,'DATA ENTRY CLOSED!!',/,18x,
   2 'Create new file for remainder of analyses!')
815 format(' ',a10,' This segment either does not exist or has no ',
   a'data!!  ENTER:',/,19x,'"0" Begin again; or "1" TERMINATE RUN.')
824 format(' ',//,'YOU ALREADY HAVE A SEGMENT (FILE) WITH THIS NAME!!'
   a ,/,15x,'Segment name = ',a10,/,
   a'Creation of the proposed segment with this name will override',/,
   b'and destroy the existing segment!  ENTER one code integer:',
   b/,5x,'"0"  RENAME proposed new segment,',/,
   c5x,'"1"  CONTINUE and destroy existing segment',/,5x,
   c'"2"  CALCULATE salt norm for the existing segment',/,5x,
   d'"3"  TERMINATE this run')
825 format(' ','Desired format of proposed input file:',
   a'  "0" = SNORM;  "1" = WATEQ')
830 format(' ','Print-out destination (ENTER one code integer):',/,8x
   a,'[Selecting "0" or "1" will allow subsequent storage selection]',
   a/,2x,'"0" Output to remote terminal with >130 spaces/line',/,2x,
   b'"1" Output to remote terminal with <130 spaces/line',/,2x,
   d'"2" Output only as segment to be stored in directory')
831 format(' ',1x,'"3" NO OUTPUT -- only creating new segment of ',
   a'input data')
835 format(' ','Storage of output as segment(s) in user''s directory'
   a,' (ENTER one code integer):')
836 format(' ',1x,'"0" No output storage desired.')
837 format(' ',1x,'"1" For subsequent spooling to line printer ',
   a'recognizing carriage control.',/,2x,
   b'"2" For subsequent spooling to output device without ',
   c'carriage control.',/,2x,'"3" Both "1" and "2" above.')
861 format(' ','ENTER ONE desired option identifier integer:',/,10x,
   a'[If entry >0, additional options can be subsequently selected]'
   a,/,3x,'"0"  NO FURTHER OPTIONS DESIRED',/,3x,
   b'"1"  Print-out of SNORM solute and salt data bank',/,3x,
   c'"2"  Salts in units other than those of water analysis',/,3x,
   d'"3"  Salt equivalencies rather than mole quantities')
862 format(' ',2x,'"4"  Dissolved nitrate recast as ammonium',/,3x,
   a'"5"  Dissolved ammonium recast as nitrate',/,3x,
   b'"6"  Dissolved nitrate replaced by bicarbonate',/,3x,
   c'"7"  Selected solutes reset to 0.0 concentration')
863 format(' ','Salt output units (enter an integer code):',/,5x,
   a'"1" Salt per kilogram of water units',/,5x,
   b'"2" Salt per kilogram of solution units',/,5x,
   c'"3" Salt per liter of solution units')
845 format(a2,a10)
847 format(' ','ENTER two-digit code number for up to ten solutes ',
   a'that must be present:'
   a //,3x,'01 Ca      02 Mg      03 Na      04 K       05 Cl',/,3x,
   b     '06 SO4    07 PO4     08 CO3     09 Li      10 NH4',/,3x,
   c     '11 NO3    12 Ba      13 Sr      14 B       15 F',/,3x,
   d     '17 HCO3   20 Br      21 I',/,
   e '--',9(1x,'--'))
848 format(a3,a10)
850 format(a12)
851 format(a13)
854 format(' ')
```

```
 855 format(' ','Your output segment with carriage control = ',al3)
 860 format(' ','Your output segment with no carriage control = ',al3)
 865 format(' ','ENTER two-digit code number for up to ten solutes ',
    a'to be set to zero:'
    a //,3x,'01 Ca      02 Mg      03 Na      04 K       05 Cl',/,3x,
    b    '06 SO4     07 PO4     08 CO3     09 Li      10 NH4',/,3x,
    c    '11 NO3     12 Ba      13 Sr      14 B       15 F',/,3x,
    d    '17 HCO3    20 Br      21 I',/,
    e '--',9(lx,'--'))
 870 format(i2,9(lx,i2))
 875 format(' ','Zero concentration set for ',a5)
 880 format(' ','Another option??',
    a'  (ENTER "0" or desired option identifier)')
 881 format(' ','Output to list solute and salt data bank')
 883 format(' ','Nitrate to be recast as ammonium')
 884 format(' ','Ammonium to be recast as nitrate')
 885 format(' ','Nitrate to be recast as bicarbonate')
 886 format(' ','Salt equivalencies rather than mole quantities.')
 888 format(' ',/,'ELECTED OPTIONS')
 889 format(' ',/,'NO OPTIONS ELECTED')
 890 format(a5,lx,f9.5,3x,i2)
 895 format(al5,a20,6(lx,i2,lx,i2))
 896 format(' ','If possible, salts in per kg-H2O units')
 897 format(' ','If possible, salts in per kg solution units')
 898 format(' ','If possible, salts in per liter solution units')
 899 format('SS.',al0)
 905 format(lx,'Give title for this group of waters'
    a ,' (up to 80 character string).')
 910 format(a80)
 920 format(lx,'Enter data for analysis no. ',i2,'.',/5x,
    a '1. sample number (up to 10 character string).',/5x,
    b '2. sample ph, 20.0 if unknown (decimal point required).',/5x,
    c '3. sample density, 0.0 if unknown (decimal point req.).',/5x,
    d '4. concentration units of analysis (integer code).',/10x,
    f '"1" = molality',/10x,
    g '"2" = mg/kg solution (ppm)',/10x,
    h '"3" = milliequivalents/liter',/10x,
    i '"4" = mg/liter',/10x,
    i '"5" = millimoles/liter',/5x,
    j '5. sample description (up to 40 character string).',/
    k '1',10x,'2',6x,'3',5x,'4',lx,'5',/
    l 10('-'),lx,6('-'),lx,5('-'),lx,'-',lx,40('-'))
 925 format(al0,lx,f6.3,lx,f5.3,lx,il,lx,a40)
 930 format(al0,2x,a40,lx,f6.3,lx,f5.3,lx,il)
 935 format(lx,'Enter analytical data for major elements',
    a ' (analysis ',i2,'):',/llx,'(decimal point required)',/,
    a'Ca',9x,'Mg',9x,'Na',9x,'K',10x,'Cl',9x,'SO4',
    b/,6(10('-'),lx))
 940 format(6ell.5)
 945 format(lx,'Enter identifier integer and data for five species',
    a ' (analysis ',i2,'):',
    a /10x,'(decimal point required in data value)',
    a     /5x,'01 CO3',10x,'05 NO3',10x,'09 NH4',
    a     /5x,'02 HCO3',9x,'06 Ba',llx,'10 PO4',
    a     /5x,'03 Li',llx,'07 Sr',llx,'11 F',
    a     /5x,'04 Br',llx,'08 B',12x,'12 I')
 950 format(5('--',lx,10('-'),lx))
 955 format(5(i2,lx,el0.4,lx))
 960 format(5(lx,i2,lx,el0.4))
 961 format(' ','All output files filled; PROGRAM TERMINATED!!',/,5x,
    a'Delete unneeded output files and reexecute SNORM!!')
 975 format(' ',20x,'ADJUST PRINTER PAGE')
 980 format(' ','ENTER:  "9" to start over',/,9x,'"8" to terminate',
    a' program',/,3x,'otherwise enter <RETURN>')
 985 format(' ','ENTER:  "9" to start over (your new data file, "',al0,
    a'", will be retained)',/,9x,'"8" to terminate',
    b' program (',10x,'"',10x,'"',10x,'"',10x,')',/,3x,
    c'otherwise enter <RETURN>')
     end
c***********************************************************************
```

```
c***********************************************************************
c                             Subroutine SALWAT
c***********************************************************************
c
c   Reading or writing data files of analyses in WATEQ format.
c
      subroutine salwat
      character*76 linet
      character*6 lwl,nul6
      character*5 lw2,nul5
      character*4 card,word
      dimension qw(7),iw(16),card(6),lwl(5),lw2(2),nul6(2),nul5(2)
      character*80 nbatch
      character*40 ndes
      character*20 mf
      character*15 nmin
      character*13 nsimp,lout,lloc
      character*10 nfile,nnum
      character*5 ncom
      common ncom(25),atw(25),nv(25),v(25),va(25),chg,kbor,nitro,np,kid,
     a ncfn,nnox,nc,cz(25,14),nnax,lout,kbri,kfile,s(99),kred,npage,kxt,
     c isalt(99),lunit,konf,nix(25),nnix,x(25),xo(25),c(25),lloc,nbatch,
     d kend,to(25),kid2,kfirst,kpage,ndes,nnum,nuts,nmin(99),kbank,kidl,
     e nfile,muts,mf(99),lc(99,6),lz(99,6),lh(99),la(99),z(99,6),ph,den,
     f must(10),nsimp,nu(10),naly(99),kid3,mp(9),mr(9),ctz(14),nax(25)
      data card/'CONC','EROR','DELH','TABL','LOGK','    '/
      data nul6/'      ','   0.0'/
      data nul5/'     ','  0.0'/
      if(konf.ne.0) go to 500
c
c         Reading and translating WATEQ input file for SNORM
c
      read(nu(2),211,end=950)nbatch
  210 continue
      kid = 1
      read(nu(2),221,err=900) (qw(i),i=1,7),(iw(i),i=1,11)
      ph = qw(2)
      den = qw(6)
      if(iw(1).eq.0) nuts = 5
      if(iw(1).eq.1) nuts = 3
      if(iw(1).eq.2) nuts = 4
      if(iw(1).eq.3) nuts = 2
      if(iw(1).eq.4) nuts = 1
      read(nu(2),231) (c(i),i=1,6)
      read(nu(2),231,err=900) (qw(i),i=1,6)
      c(18) = qw(1)
      c(7) = qw(4)
      c(13) = qw(5)
      c(15) = qw(6)
      if(iw(10).ne.0) read(nu(2),235) word,linet
      if(iw(11).ne.0) read(nu(2),235) word,linet
  240 continue
      do 280 j=1,100
      read(nu(2),241,err=900) word,(iw(i),qw(i),i=1,5)
      if(word.eq.card(6)) go to 300
      if(word.ne.card(1)) go to 280
      do 270 i=1,5
      if(iw(i).eq.0) go to 280
      if(iw(i).eq.18) c(8) = qw(i)
      if(iw(i).eq.39) c(10) = qw(i)
      if(iw(i).eq.81) c(9) = qw(i)
      if(iw(i).eq.85) c(11) = qw(i)
      if(iw(i).eq.87) c(14) = qw(i)
      if(iw(i).eq.90) c(12) = qw(i)
      if(iw(i).eq.98) c(16) = qw(i)
  270 continue
  280 continue
  300 continue
      go to 990
c
c                Creating input file in WATEQ format
c
  500 continue
      nnnn = 1
      go to 502
  501 continue
      kid = 1
```

```
c                                         Title, job description "TITL"
      print 601
      read 600,i
      if(i.eq.1) go to 990
      nnnn = nnnn + 1
      if(nnnn.lt.100) go to 502
      print 645
      go to 990
  502 continue
      print 602
      read 604,nbatch
      print 604,nbatch
      print 605
      read 600,i
      if(i.eq.1) go to 502
      write(nu(1),604)nbatch
c                                  TEMP, PH, EHM, EHMC, EMFZ, DENS, DOX
  503 continue
      print 606
      read(nu(10),607,err=505) (lw1(i),i=1,5),(lw2(i),i=1,2)
      do 504 i=1,5
      if(lw1(i).eq.nul6(1)) lw1(i) = nul6(2)
      if(i.gt.2) go to 504
      if(lw2(i).eq.nul5(1)) lw2(i) = nul5(2)
  504 continue
      go to 506
  505 continue
      print 603
      go to 503
  506 continue
      print 607,(lw1(i),i=1,5),(lw2(i),i=1,2)
      print 605
      read 600,i
      if(i.eq.1) go to 503
c            FLAG, CORALK, PECALC, IGO, PRT(1 to 4), IDAVES, ISPEC, IMIN
  507 continue
      print 608
      read(nu(10),609,err=508) (iw(i),i=1,11)
      go to 509
  508 continue
      print 603
      go to 507
  509 continue
      print 609,(iw(i),i=1,11)
      print 605
      read 600,i
      if(i.eq.1) go to 507
      write(nu(1),610,err=504) (lw1(i),i=1,5),
     a(lw2(i),i=1,2),(iw(i),i=1,11)
      j10 = iw(10)
      j11 = iw(11)
c                          Solute concentrations (Ca, Mg, Na, K, Cl, SO4)
  511 continue
      print 611
      read(nu(10),612,err=512) (qw(i),i=1,6)
      go to 513
  512 continue
      print 603
      go to 511
  513 continue
      print 612,(qw(i),i=1,6)
      print 605
      read 600,i
      if(i.eq.1) go to 511
      write(nu(1),612,err=512) (qw(i),i=1,6)
c                      Solute concentrations (HCO3, SiO2, Fe, PO4, Sr, F)
  515 continue
      print 613
      read(nu(10),612,err=516) (qw(i),i=1,6)
      go to 517
  516 continue
      print 603
      go to 515
  517 continue
      print 612,(qw(i),i=1,6)
      print 605
      read 600,i
      if(i.ne.0) go to 515
```

```
      write(nu(1),612,err=516) (qw(i),i=1,6)
c                           Aqueous species selected for output  "KSPEC(i)"
  521 continue
      if(j10.eq.0) go to 525
      print 615,j10
      read(nu(10),616,err=522) (iw(i),i=1,16)
      go to 523
  522 continue
      print 603
      go to 521
  523 continue
      print 616,(iw(i),i=1,16)
      print 605
      read 600,i
      if(i.ne.0) go to 521
      write(nu(1),616,err=522) (iw(i),i=1,16)
c                                   Minerals selected for output  "KMIN(i)"
  525 continue
      if(j11.eq.0) go to 531
      print 617,j11
      read(nu(10),616,err=526) (iw(i),i=1,16)
      go to 527
  526 continue
      print 603
      go to 525
  527 continue
      print 616,(iw(i),i=1,16)
      print 605
      read 600,i
      if(i.eq.1) go to 525
      write(nu(1),616,err=526) (iw(i),i=1,16)
c                                   Concentrations of other solutes  "CONC"
  531 continue
      print 620
      read 600,i
      if(i.eq.1) go to 535
  534 continue
      print 621
      read(nu(10),622,err=532) (iw(i),qw(i),i=1,5)
      go to 533
  532 continue
      print 603
      go to 534
  533 continue
      print 622,(iw(i),qw(i),i=1,5)
      print 605
      read 600,i
      if(i.eq.1) go to 534
      word = card(1)
      write(nu(1),623,err=532) word,(iw(i),qw(i),i=1,5)
      if(iw(5).ne.0) go to 531
c                              Overrides preset balance constraints  "EROR"
  535 continue
      print 625
      read 600,i
      if(i.eq.0) go to 540
  538 continue
      print 626
      read(nu(10),622,err=536) (iw(i),qw(i),i=1,5)
      go to 537
  536 continue
      print 603
      go to 538
  537 continue
      print 622,(iw(i),qw(i),i=1,5)
      print 605
      read 600,i
      if(i.ne.0) go to 538
      word = card(2)
      write(nu(1),623,err=536) word,(iw(i),qw(i),i=1,5)
c                            Overrides standard reaction enthalpies  "DELH"
  540 continue
      print 630
      read 600,i
      if(i.eq.0) go to 545
  541 continue
      print 631
      read(nu(10),622,err=542) (iw(i),qw(i),i=1,5)
```

```
      go to 543
  542 continue
      print 603
      go to 541
  543 continue
      print 622,(iw(i),qw(i),i=1,5)
      print 605
      read 600,i
      if(i.ne.0) go to 541
      word = card(3)
      write(nu(1),623,err=542) word,(iw(i),qw(i),i=1,5)
      if(iw(5).ne.0) go to 541
c                                    Overrides log K's of reaction  "TABL"
  545 continue
      print 633
      read 600,i
      if(i.eq.0) go to 550
  546 continue
      print 634
      read(nu(10),622,err=547) (iw(i),qw(i),i=1,5)
      go to 548
  547 read 603
      go to 546
  548 continue
      print 622,(iw(i),qw(i),i=1,5)
      print 605
      read 600,i
      if(i.ne.0) go to 546
      word = card(4)
      write(nu(1),623,err=547) word,(iw(i),qw(i),i=1,5)
      if(iw(5).ne.0) go to 545
c                                           Overrides log K's vs T  "LOGK"
  550 continue
      print 637
      read 600,i
      if(i.eq.0) go to 555
  551 continue
      print 638
      read(nu(10),622,err=552) (iw(i),qw(i),i=1,5)
      go to 553
  552 continue
      print 603
      go to 551
  553 continue
      print 622,(iw(i),qw(i),i=1,5)
      print 605
      read 600,i
      if(i.ne.0) go to 551
      word = card(5)
      write(nu(1),623,err=552) word,(iw(i),qw(i),i=1,5)
      go to 550
c                                           End of input for this analysis
  555 continue
      word = card(6)
      write(nu(1),640) word
      go to 501
  900 continue
      kid3 = 1
  950 continue
      kend = 1
  990 continue
      return
  211 format(a80)
  221 format(5(f6.0,1x),2f5.0,1x,9i1,2i3)
  231 format(6(e12.5))
  235 format(a4,a76)
  241 format(a4,1x,5(i3,e12.5))
  600 format(i1)
  601 format(' ','Another water??   "0" = Yes;  "1" = No.')
  602 format(' ','Enter sample description (up to 80 character string)')
  603 format(' ','INPUT ERROR -- reenter these data')
  604 format(a80)
  605 format(' ','IS THIS CORRECT??   "0" = Yes;  "1" = No.')
  606 format(' ','ENTER: A. Temperature (deg. C).',/,8x,'B. pH.',/,6x,
     a'C-E. Eh data (see WATEQ documentation).',/,8x,
     a'F. Density (g/cc).',/,
     b8x,'G. Dissolved oxygen (mg/l).',/,15x,'[Decimal point with each]'
     c,/,'A',6x,'B',6x,'C',6x,'D',6x,'E',6x,'F',5x,'G',/,
```

```
     d5(6('-'),1x),2(5('-'),1x))
  607 format(5(a6,1x),2(a5,1x))
  697 format(5(f6.0,1x),2(f5.0,1x))
  608 format(' ','ENTER: A. Input concentrations ("0" = mmole/l; ',
     a'"1" = meq/l;',/,11x,'"2" = mg/l; "3" = ppm; "4" = molality)',/,
     b 8x,'B. Alkalinity method (See WATEQ documentation)',/,8x,
     c'C. Redox method (See WATEQ documentation)',/,8x,
     d'D. Input error options (See WATEQ documentation)',/,6x,
     e'E-H. Output deletion options (See WATEQ documentation)',/,8x,
     f'I. Ion-pair activity coefficients (See WATEQ documentation)',/,
     g8x,'J. Restricting output species (See WATEQ documentation)',/,
     h8x,'K. Restricting output minerals (See WATEQ documentation)',/,
     i15x,'[All right justified integer values]',
     j/,'A B C D E F G H I   J   K',/,9('-',1x),'---',1x,'---')
  609 format(9(i1,1x),i3,1x,i3)
  610 format(5(a6,1x),2a5,1x,9i1,2i3)
  611 format(' ','ENTER CONCENTRATIONS: [decimal point required]',/,
     a'Ca',10x,'Mg',10x,'Na',10x,'K',11x,'Cl',10x,'SO4',/,
     b6(11('-'),1x))
  612 format(6e12.5)
  613 format(' ','ENTER CONCENTRATIONS: [decimal point required]',/,
     a'HCO3',8x,'SiO2',8x,'Fe',10x,'PO4',9x,'Sr',10x,'F',/,
     b6(11('-'),1x))
  615 format(' ','ENTER ',i3,' index numbers of specified species',
     a' in output listing.',/,15x,'[right-justified integers]',/,
     b16(2x,'---'))
  616 format(16i5)
  617 format(' ','ENTER ',i3,' index numbers of specified minerals',
     a' in output listing.',/,15x,'[right-justified integers]',/,
     b16(2x,'---'))
  620 format(' ','Any additional solutes??   "0" = Yes; "1" = No',
     a/,5x,'"CONC" card(s) in WATEQ')
  621 format(' ','ENTER index integer and concentration [decimal',
     a' point] for each in analysis:',/,
     b5x,'017 H2S',5x,'018 CO3',5x,'039 NH4',5x,'051 Al',/,
     c5x,'081 Li ',5x,'085 NO3',5x,'086 H2CO3',3x,'087 B',/,
     d5x,'090 Ba ',5x,'098 Br ',5x,'101 Mn',/,
     e5(3('-'),1x,9('-'),3x))
  622 format(5(i3,e12.5,1x))
  623 format(a4,1x,5(i3,e12.5))
  625 format(' ','Any override of mass balance convergence',
     a' constraints (WATEQ "EROR" card)?',/,12x,'"0" = no; "1" = Yes')
  626 format(' ','ENTER reset values [decimal point] for:',/,
     a4x,'Carbon',10x,'Sulfate',9x,'Fluoride',8x,'Phosphate',7x,
     b'Chloride',/,4x,4(9('-'),7x),9('-'))
  630 format(' ','Any override of standard enthalpies?? "0" = No; '
     b,'"1" = Yes (WATEQ "DELH" card)')
  631 format(' ','ENTER reaction index number [right-justified integer]'
     a,/,7x,'and the new enthalpy value [decimal point]',/,
     b5(3('-'),1x,9('-'),3x))
  633 format(' ','Any overrides of reaction constants??  "0" = No;'
     a,' "1" = Yes  (WATEQ "TABL" card)')
  634 format(' ','ENTER reaction index number [right-justified',
     a' integer]',/7x,'and new reaction constant [decimal point].',/,
     b5(3('-'),1x,9('-'),3x))
  637 format(' ','Any overrides of log k vs. T constants??  "0" = No;',
     b' "1" = Yes',/,15x,'WATEQ "LOGK" card)')
  638 format(' ','ENTER reaction index number [right-justified',
     a' integer]',/,7x,'and five new constants [decimal point',
     b' with each]',/,3('-'),1x,9('-'),4(7x,9('-')))
  640 format(a4)
  645 format(' ',16x,'99 analyses entered in file -- file full!',/,
     1 28x,'DATA ENTRY CLOSED!!',/,18x,
     2 'Create new file for remainder of analyses!!')
      end
c***********************************************************************
```

```
c***********************************************************************
c                         Subroutine LOAD
c***********************************************************************
c
c   Reading a single analysis for the salt norm calculation; recasting
c   analytical data into alternative concentration units; calculating
c   CO3-HCO3 speciation if necessary.
c
```

```
      subroutine load
      dimension cc(5),ic(5)
      character*80 nbatch
      character*40 ndes
      character*20 mf
      character*15 nmin
      character*13 nsimp,lout,lloc
      character*10 nfile,nnum
      character*5 ncom
      common ncom(25),atw(25),nv(25),v(25),va(25),chg,kbor,nitro,np,kid,
     a ncfn,nnox,nc,cz(25,14),nnax,lout,kbri,kfile,s(99),kred,npage,kxt,
     c isalt(99),lunit,konf,nix(25),nnix,x(25),xo(25),c(25),lloc,nbatch,
     d kend,to(25),kid2,kfirst,kpage,ndes,nnum,nuts,nmin(99),kbank,kidl,
     e nfile,muts,mf(99),lc(99,6),lz(99,6),lh(99),la(99),z(99,6),ph,den,
     f must(10),nsimp,nu(10),naly(99),kid3,mp(9),mr(9),ctz(14),nax(25)
      kid2 = 0
      do 100    i=1,nc
      c(i) = 0.0
      xo(i) = 0.0
      to(i) = 0.0
  100 continue
c
c                  Reading in analysis data
c
      kend = 0
      nnox = 1
      kxt = 0
      kid3 = 0
      if(kidl.ne.0) go to 103
      read(nu(2),101) nbatch
      if(mp(5).eq.1) write(nu(7),101) nbatch
      if(kid.eq.0) go to 110
      rewind(nu(2))
      call salwat
      go to 190
  103 continue
      if(kid.eq.0) go to 110
      call salwat
      go to 190
  110 continue
c                                         Sample number and description
      read(nu(2),111,err=120,end=900) nnum,ndes,ph,den,nuts
      if(kidl.eq.0.and.nuts.eq.0) go to 120
      go to 125
  120 continue
      if(kidl.ne.0) go to 890
      rewind nu(2)
      call salwat
      go to 190
  125 continue
      if(nuts.eq.0) go to 900
c                                                 Major component data
      read(nu(2),121,err=890,end=900) (c(i),i=1,6)
c                                                 Other conponent data
  130 continue
      do 135    i=1,5
      ic(i) = 0
      cc(i) = 0.0
      if(i.lt.4) mr(i) = 0
  135 continue
      read(nu(2),131,err=890,end=190) (ic(i),cc(i),i=1,5)
      do 180 i=1,5
      if(ic(i).eq.0) go to 190
      if(ic(i).eq.20) ic(i) = 15
      if(ic(i).eq.10) ic(i) = 16
      if(ic(i).eq.18) ic(i) = 10
      if(ic(i).eq.19) ic(i) = 7
      if(ic(i).eq.17) ic(i) = 18
      if(ic(i).eq.21) ic(i) = 17
  150 continue
      c(ic(i)) = cc(i)
      cc(i) = 0.0
  180 continue
      go to 130
  190 continue
      if(mp(9).eq.0) go to 195
      do 193 i=1,nc
      if(c(i).gt.0.0) go to 193
```

```
      do 192 j=1,10
      if(must(j).eq.i) go to 250
  192 continue
  193 continue
  195 continue
      if(kend.eq.1) go to 900
      if(kid3.eq.1) go to 900
      if(nuts.gt.2) kxt = 1
      muts = 1
      if(nuts.gt.2) muts = 2
      if(kred.ne.1) go to 200
      if(nuts.eq.3.and.den.gt.0.0) muts = 3
      if(nuts.gt.3.and.den.gt.0.0) muts = 4
  200 continue
      if(kred.ne.2) go to 205
      if(nuts.eq.3.and.den.gt.0.0) muts = 5
      if(nuts.gt.3.and.den.gt.0.0) muts = 6
  205 continue
      if(kred.ne.3) go to 210
      if(nuts.eq.1) muts = 7
      if(nuts.eq.2) muts = 8
  210 continue
c
c                                  Requested deletions and replacements
c
      n = kid1 + 1
      if(n.eq.100) n = 99
      if(naly(n).eq.0) go to 250
      nnax = 0
      k = nnix + nitro + ncfn
      if(k.eq.0) go to 300
      jump = 0
      mp(2) = 0
      mp(3) = 0
      if(nitro.eq.0) go to 220
      if(nitro.eq.1.and.c(11).gt.0.0) mp(2) = 1
      if(nitro.eq.2.and.c(10).gt.0.0) mp(2) = 2
  220 continue
      if(ncfn.eq.0) go to 240
      if(c(11).gt.0.0.and.nitro.ne.1) mp(3) = 1
      if(c(10).gt.0.0.and.nitro.eq.2) mp(3) = 1
  240 continue
      if(mp(2).ne.0.or.mp(3).ne.0) go to 300
      do 250 i=1,nc
      if(nix(i).eq.0) go to 250
      if(c(i).gt.0.0) go to 300
      if(i.eq.8.and.c(18).gt.0.0) go to 300
      if(i.eq.17.and.c(8).gt.0.0) go to 300
  250 continue
      nnox = 0
      go to 990
c
c                   0 set of analytical variables
c
  300 continue
      do 320 k=1,14
      ctz(k) = 0.0
      do 315 i=1,25
      cz(i,k) = 0.0
  315 continue
  320 continue
      v(14) = -7.0/12.0
      va(14) = abs(v(14))
c
c                Original analytical data recast to several units
c
c                                          Original analyses: molality
      if(nuts.ne.1) go to 420
      do 410    i=1,nc
      if(c(i).eq.0.0) go to 410
      cz(i,1) = c(i)
      ctz(1) = ctz(1) + cz(i,1)
      xo(i) = cz(i,1)
      cz(i,2) = (xo(i) * atw(i)) * 1000.0
      ctz(2) = ctz(2) + cz(i,2)
  410 continue
      q = 1000.0 / (1000.0 + (ctz(2)/1000.0))
      do 415 i=1,nc
```

```
      if(cz(i,2).eq.0.0) go to 415
      cz(i,2) = cz(i,2) * q
  415 continue
      ctz(2) = ctz(2) * q
      go to 480
  420 continue
c                                     Original analyses: mg/kg solution
      if(nuts.ne.2) go to 440
      do 430 i=1,nc
      if(c(i).eq.0.0) go to 430
      cz(i,2) =  c(i)
      ctz(2) = ctz(2) + cz(i,2)
  430 continue
      q = 1000.0 / (1000.0 - (ctz(2) / 1000.0))
      do 435    i=1,nc
      if(cz(i,2).eq.0.0) go to 435
      cz(i,1) =  q * (cz(i,2) / (1000.0 * atw(i)))
      xo(i) =  cz(i,1)
      ctz(1) = ctz(1) + cz(i,1)
  435 continue
      go to 480
  440 continue
c                           Original analyses: meq/liter or mmoles/liter
      if(nuts.ne.3.and.nuts.ne.5) go to 460
      do 450 i=1,nc
      if(c(i).eq.0.0) go to 450
      if(nuts.eq.3) cz(i,3) = c(i)
      if(nuts.eq.5) cz(i,5) = c(i)
      if(nuts.eq.3) cz(i,5) = cz(i,3) / va(i)
      if(nuts.eq.5) cz(i,3) = cz(i,5) * va(i)
      cz(i,4) = cz(i,5) * atw(i)
      xo(i) = cz(i,5) / 1000.0
      cz(i,4) = xo(i) * atw(i) * 1000.0
      ctz(3) = ctz(3) + cz(i,3)
      ctz(4) = ctz(4) + cz(i,4)
      ctz(5) = ctz(5) + cz(i,5)
  450 continue
      go to 480
  460 continue
c                                          Original analyses: mg/liter
      do 470 i=1,nc
      if(c(i).eq.0.0) go to 470
      cz(i,4) = c(i)
      cz(i,5) = c(i) / atw(i)
      ctz(4) = ctz(4) + cz(i,4)
      xo(i) = cz(i,4) / (atw(i) * 1000.0)
      cz(i,3) = 1000.0 * (xo(i) * va(i))
      ctz(3) = ctz(3) + cz(i,3)
      ctz(5) = ctz(5) + cz(i,5)
  470 continue
  480 continue
      do 475 i=1,nc
      to(i) = xo(i)
  475 continue
      if(den.eq.0.0) go to 500
c                                         Kg units to/from liter units
      if(nuts.gt.2) go to 490
      do 485 i=1,nc
      if(xo(i).eq.0.0) go to 485
      cz(i,4) = cz(i,2) * den
      cz(i,3) = (cz(i,4) * va(i)) / atw(i)
      cz(i,5) = cz(i,4) / atw(i)
      ctz(3) = ctz(3) + cz(i,3)
      ctz(4) = ctz(4) + cz(i,4)
      ctz(5) = ctz(5) + cz(i,5)
  485 continue
      go to 500
  490 continue
      sumt = 1000.0 * den
      sumw = sumt - (ctz(4) / 1000.0)
      q = 1000.0 / sumw
      r = 1000.0 / sumt
      do 495 i=1,nc
      if(xo(i).eq.0.0) go to 495
      cz(i,2) = cz(i,4) / den
      cz(i,1) = xo(i) * q
      ctz(2) = ctz(2) + cz(i,2)
      ctz(1) = ctz(1) + cz(i,1)
```

```
  495 continue
  500 continue
      if(ctz(1).eq.0.0) go to 510
      do 505 i=1,nc
      cz(i,6) = cz(i,1)*atw(i)
      cz(i,7) = cz(i,2)/(1000.0*atw(i))
      ctz(6) = ctz(6) + cz(i,6)
      ctz(7) = ctz(7) + cz(i,7)
  505 continue
  510 continue
c                                                     Carbonate speciation
      if(ph.gt.19.0) go to 520
      if(xo(8).gt.0.0.and.xo(18).gt.0.0) go to 520
      dcon = 1.0
      if(ctz(1).ne.0.0) go to 514
      q = 0.0
      do 511 i=1,nc
      if(v(i).le.0.0.or.xo(i).eq.0.0) go to 511
      q = q + (xo(i)*v(i))
  511 continue
      dcon = 1.0 + (0.022*q)
  514 continue
      qis = 0.0
      do 516 i=1,nc
      if(xo(i).eq.0.0) go to 516
      if(ctz(1).ne.0.0) qz = cz(i,1)*va(i)*va(i)
      if(ctz(1).eq.0.0) qz = xo(i)*dcon*va(i)*va(i)
      qis = qis + (qz*0.5)
  516 continue
      a = 0.5108639
      b = 0.3286506
      cdh = 5.4
      q = sqrt(qis)
      zap = -(a*q)/(1.0 + (b*cdh*q))
      grat = (10.0**zap)/(10.0**(4.0*zap))
      q = (grat*(10.0**(-10.329)))/(10.0**(-ph))
      zap = q/(1.0 + q)
      if(zap.lt.0.001) go to 520
      sum = xo(8) + xo(18)
      xo(8) = zap*sum
      xo(18) = sum - xo(8)
  520 continue
c                                                     Nitrogen reassigment
      if(xo(10).eq.0.0.and.xo(11).eq.0.0) go to 630
      if(nitro.eq.0) go to 620
      if(nitro.eq.2) go to 610
      xo(10) = xo(10) + xo(11)
      xo(11) = 0.0
      go to 620
  610 continue
      xo(11) = xo(10) + xo(11)
      xo(10) = 0.0
  620 continue
      if(ncfn.eq.0.or.xo(11).eq.0.0) go to 630
      xo(18) = xo(18) + xo(11)
      xo(11) = 0.0
  630 continue
      go to 990
  890 continue
      kid3 = 1
  900 continue
      kend = 1
  990 continue
      return
  101 format(a80)
  102 format('SS.',a10)
  111 format(a10,2x,a40,1x,f6.3,1x,f5.3,1x,i1)
  121 format(6e11.5)
  131 format(5(1x,i2,1x,e10.4))
      end
c*************************************************************************
```

```fortran
c***********************************************************************
c                         Subroutine JOIN
c***********************************************************************
c
c   Determining adjusted solute concentrations, basic parameters of
c   normative salt assemblage, all possible permissable assemblages of
c   co-existing salts, the unique assemblage with no negative abundance,
c   its recasting to the salt norm, and the simple salt assemblage.
c
      subroutine join
      double precision dal,dxc
      dimension dal(196),dxc(14),nono(30,4),mv(55),lx(25),na(15),nan(6),
     a nann(6),max(14),min(14),konk(4),al(196),xcc(14),ss(14),am(14,14),
     b mm(14),m(55)
      character*80 nbatch
      character*40 ndes
      character*20 mf
      character*15 nmin
      character*13 nsimp,lout,lloc
      character*10 nfile,nnum
      character*5 ncom
      common ncom(25),atw(25),nv(25),v(25),va(25),chg,kbor,nitro,np,kid,
     a ncfn,nnox,nc,cz(25,14),nnax,lout,kbri,kfile,s(99),kred,npage,kxt,
     c isalt(99),lunit,konf,nix(25),nnix,x(25),xo(25),c(25),lloc,nbatch,
     d kend,to(25),kid2,kfirst,kpage,ndes,nnum,nuts,nmin(99),kbank,kidl,
     e nfile,muts,mf(99),lc(99,6),lz(99,6),lh(99),la(99),z(99,6),ph,den,
     f must(10),nsimp,nu(10),naly(99),kid3,mp(9),mr(9),ctz(14),nax(25)
      data nono/4,5,6,8,9,13,14,15,16,18,19,20,23,41,44,46,49,50,53,
     a 11*99,25,26,27,31,32,35,36,39,40,21*99,11,12,15,16,17,18,
     b 19,21,28,43,44,45,47,48,16*99,4,5,6,7,8,9,10,49,50,53,20*99/
      jump = 0
      nbase = 55
c
c              Borate charge and salt composition assignment
c
      kbor = 0
      if(xo(14).gt.0.0) kbor = -1
      if(kbor.eq.0) go to 220
  100 continue
      if(kbor.gt.0) go to 170
      v(14) = -7.0/12.0
      z(43,1) = 77.0/43.0
      z(43,2) = 264.0/43.0
      z(44,1) = 126./129.0
      z(44,2) = z(44,1)
      z(44,3) = 216.0/43.0
      z(45,1) = z(43,1)
      z(45,2) = z(43,2)
      z(46,1) = 98.0/43.0
      z(46,2) = 168.0/43.0
      do 160 i=43,46
      ik = i + 14
      do 150 k=1,lh(i)
      z(ik,k) = z(i,k)
  150 continue
  160 continue
      go to 200
  170 continue
      if(kbor.eq.1) v(14) = -0.6
      if(kbor.eq.2) v(14) = -2.0/3.0
      if(kbor.eq.4) v(14) = -0.5
      do 190 i=43,46
      do 180 k=1,5
      if(k.gt.lh(i)) go tol90
      z(i,k) = float(lz(i,k))
  180 continue
  190 continue
  200 continue
      va(14) = abs(v(14))
  220 continue
c
c                Cation-anion charge balance adjustment
c
c                         Concentration of requested solutes set to zero
      nnax = 0
      spos = 0.0
      sneg = 0.0
      do 230 i=1,nc
```

```
      x(i) = 0.0
      c(i) = 0.0
      nax(i) = 0
      if(xo(i).gt.0.0.and.nix(i).eq.1) nax(i) = 1
      if(xo(i).eq.0.0.or.nax(i).eq.1) go to 230
      if(v(i).gt.0.0) spos = spos + (xo(i)*va(i))
      if(v(i).lt.0.0) sneg = sneg + (xo(i)*va(i))
  230 continue
      chg = spos/sneg
      achg = (spos + sneg)/2.0
      rpos = achg/spos
      rneg = achg/sneg
      do 240 i=1,nc
      if(nax(i).eq.1) nnax = 1
      if(xo(i).eq.0.0.or.nax(i).eq.1) go to 240
      if(v(i).gt.0.0) x(i) = xo(i)*rpos
      if(v(i).lt.0.0) x(i) = xo(i)*rneg
      if(v(i).eq.0.0) x(i) = xo(i)
      c(i) = x(i)
  240 continue
      kbri = 0
      if(x(16).eq.0.0.and.x(17).eq.0.0) go to 245
      x(5) = x(5) + x(16) + x(17)
      x(16) = 0.0
      x(17) = 0.0
      kbri = 1
  245 continue
      x(8) = x(8) + (0.5 * x(18))
      x(18) = 0.0
      if(kbor.gt.0.or.kbor.eq.-2) go to 595
c
c              Establishing parameters for nested do-loop sequence
c
c                                 Determining major character of salt norm
      do 290 i=1,4
      konk(i) = 0
  290 continue
      qn1 = (3.0*x(7))+(2.0*(x(6)+x(8)))+x(15)+(va(14)*x(14))
      qn2 = (2.0*(x(1)+x(2)+x(12)+x(13)))+x(9)
      if(qn1.gt.qn2) go to 300
      konk(1) = 1
      go to 305
  300 continue
      konk(2) = 1
      qn1 = (3.0*x(7))+(2.0*x(8))
      qn2 = 2.0*(x(1)+x(2)+x(13))
      if(qn1.gt.qn2) konk(3) = 1
      qn1 = (3.0*x(7))+(2.0*x(8))+x(15)
      qn2 = 2.0*(x(1)+x(2))
      if(qn1.lt.qn2) konk(4) = 1
  305 continue
c    Defining anion groups and base salts elegible for salt norm
      ktot = 0
      do 310 i=1,nbase
      m(i) = 0
      mv(i) = 0
      if(i.gt.14) go to 310
      mm(i) = 0
      if(i.gt.7) go to 310
      nan(i) = 0
      if(konk(2).eq.0) go to 315
      q = x(12) + x(13)
      if(q.le.x(6)) go to 315
      nono(4,2) = 27
      nono(5,2) = 27
      nono(8,2) = 99
      nono(9,2) = 99
  315 continue
  310 continue
      do 350 i=1,nbase
      do 325 k=1,4
      if(konk(k).eq.0) go to 325
      do 320 j=1,30
      if(nono(j,k).gt.i) go to 325
      if(nono(j,k).eq.i) go to 350
  320 continue
  325 continue
      do 330 k=1,la(i)
```

```
      if(lc(i,k).gt.15) go to 330
      if(x(lc(i,k)).eq.0.0) go to 350
  330 continue
      ktot = ktot + 1
      mv(ktot) = i
      if(i.lt.11) nan(1) = nan(1) + 1
      if(i.gt.10.and.i.lt.25) nan(2) = nan(2) + 1
      if(i.gt.24.and.i.lt.35) nan(3) = nan(3) + 1
      if(i.gt.34.and.i.lt.43) nan(4) = nan(4) + 1
      if(i.gt.42.and.i.lt.47) nan(5) = nan(5) + 1
      if(i.gt.46) nan(6) = nan(6) + 1
  350 continue
      if(ktot.eq.0) go to 899
c                    Designating solutes and anion groups in analysis
      nca = 0
      do 360 i=1,15
      if(x(i).eq.0.0) go to 360
      nca = nca + 1
      na(nca) = i
  360 continue
      minmax = nca - 1
      k = 0
      nant = 0
      do 370 i=1,6
      if(nan(i).eq.0) go to 370
      nant = nant + 1
      nann(nant) = nan(i)
  370 continue
c              Defining indexing limits for each loop in nested series
      max(1) = ktot - (minmax - 1)
      min(1) = 1
      do 380 i=2,minmax
      k = i - 1
      min(i) = min(k) + 1
      max(i) = max(k) + 1
  380 continue
      nsum = 0
      do 400 i=1,nant
      nsum = nsum + nann(i)
      if(max(i).gt.nsum) max(i) = nsum
  400 continue
      nsum = ktot + 1
      ii = nant
      ik = minmax
      do 410 i=1,nant
      j = nsum - nann(ii)
      if(j.gt.min(ik))  min(ik) = j
      nsum = j
      ii = ii - 1
      ik = ik - 1
  410 continue
      do 420 i=1,minmax
      if(min(i).gt.max(i)) min(i) = max(i)
  420 continue
c
c           Nested do-loops defining potential salt assemblage
c
      min1 = min(1)
      do 895 i1=min1,max(1)
      call pick(mr(1),1,i1,min2,min(2),m,mm,mv(i1),jump,minmax)
      if(jump) 500,495,895
  495 continue
      do 890 i2=min2,max(2)
      call pick(mr(1),2,i2,min3,min(3),m,mm,mv(i2),jump,minmax)
      if(jump) 500,490,890
  490 continue
      do 885 i3=min3,max(3)
      call pick(mr(1),3,i3,min4,min(4),m,mm,mv(i3),jump,minmax)
      if(jump) 500,485,885
  485 continue
      do 880 i4=min4,max(4)
      call pick(mr(1),4,i4,min5,min(5),m,mm,mv(i4),jump,minmax)
      if(jump) 500,480,880
  480 continue
      do 875 i5=min5,max(5)
      call pick(mr(1),5,i5,min6,min(6),m,mm,mv(i5),jump,minmax)
      if(jump) 500,475,875
  475 continue
```

```
      do 870 i6=min6,max(6)
      call pick(mr(1),6,i6,min7,min(7),m,mm,mv(i6),jump,minmax)
      if(jump) 500,470,870
  470 continue
      do 865 i7=min7,max(7)
      call pick(mr(1),7,i7,min8,min(8),m,mm,mv(i7),jump,minmax)
      if(jump) 500,465,865
  465 continue
      do 860 i8=min8,max(8)
      call pick(mr(1),8,i8,min9,min(9),m,mm,mv(i8),jump,minmax)
      if(jump) 500,460,860
  460 continue
      do 855 i9=min9,max(9)
      call pick(mr(1),9,i9,min10,min(10),m,mm,mv(i9),jump,minmax)
      if(jump) 500,455,855
  455 continue
      do 850 i10=min10,max(10)
      call pick(mr(1),10,i10,min11,min(11),m,mm,mv(i10),jump,minmax)
      if(jump) 500,450,850
  450 continue
      do 845 i11=min11,max(11)
      call pick(mr(1),11,i11,min12,min(12),m,mm,mv(i11),jump,minmax)
      if(jump) 500,445,845
  445 continue
      do 840 i12=min12,max(12)
      call pick(mr(1),12,i12,min13,min(13),m,mm,mv(i12),jump,minmax)
      if(jump) 500,440,840
  440 continue
      do 835 i13=min13,max(13)
      call pick(mr(1),13,i13,min14,min(14),m,mm,mv(i13),jump,minmax)
      if(jump) 500,435,835
  435 continue
      do 830 i14=min14,max(14)
      call pick(mr(1),14,i14,0,0,m,mm,mv(i14),jump,minmax)
      if(jump) 500,430,830
  430 continue
c
c               Rejecting assemblage not containing all solutes
c
  500 continue
      mr(2) = mr(2) + 1
      do 560 i=1,nc
      lx(i) = 0
  560 continue
      do 580 i=1,minmax
      do 570 k=1,lh(mm(i))
      kk = lc(mm(i),k)
      lx(kk) = 1
  570 continue
  580 continue
      do 590 i=1,nc
      if(i.gt.15) go to 595
      if(x(i).gt.0.0.and.lx(i).eq.0) go to 800
      if(x(i).eq.0.0.and.lx(i).eq.1) go to 800
  590 continue
  595 continue
c                                     Constructing minmax x minmax matrix
      do 605 i=1,196
      al(i) = 0.0
      dal(i) = 0.0
      if(i.gt.99) go to 605
      s(i) = 0.0
      if(i.gt.14) go to 605
      xcc(i) = 0.0
      dxc(i) = 0.0
      ss(i) = 0.0
      do 600 k=1,14
      am(k,i) = 0.0
  600 continue
  605 continue
      if(x(7).gt.0.0) nomit = 7
      if(x(15).gt.0.0) nomit = 15
      if(x(14).gt.0.0) nomit = 14
      if(x(11).gt.0.0) nomit = 11
      if(x(8).gt.0.0) nomit = 8
      if(x(6).gt.0.0) nomit = 6
      if(x(5).gt.0.0) nomit = 5
      ii = 0
```

```
      do 640 i=1,nca
      if(na(i).eq.nomit) go to 640
      ii = ii + 1
      xcc(ii) = x(na(i))
      do 630 k=1,minmax
      am(ii,k) = 0.0
      do 610 j=1,lh(mm(k))
      if(lc(mm(k),j).eq.na(i)) go to 620
  610 continue
      go to 630
  620 continue
      am(ii,k) = z(mm(k),j)
  630 continue
  640 continue
      ncb = ii
      mincom = minmax*minmax
      mr(3) = mr(3) + 1
c
c                            Matrix inversion
c
      call array(2,ncb,minmax,14,14,al,am)
      call convt(mincom,1,1,al,dal,0)
      call convt(ncb,1,1,xcc,dxc,0)
      call dgelg(dxc,dal,ncb,1,1.e-10,ier)
c                             Rejecting norm if negative salt quantities
      if(ier.ne.0) go to 790
      do 650 i=1,minmax
      if(dxc(i).eq.0.0) go to 650
      kix = 0
      do 645 j = 1,la(mm(i))
      if(lc(mm(i),j).gt.15) go to 645
      q = (dxc(i) * z(mm(i),j))/x(lc(mm(i),j))
      if(q.gt.1.0e-6.or.q.lt.-1.0e-6) kix = 1
  645 continue
      if(kix.eq.0) dxc(i) = 0.0
      if(dxc(i).lt.0.0) go to 790
  650 continue
c                                                      Borate evaluation
      if(kbor.ne.-1) go to 660
      jbor = 0
      if(m(43).eq.1.or.m(45).eq.1) jbor = 2
      if(m(44).eq.1) jbor = jbor + 1
      if(m(46).eq.1) jbor = jbor + 4
      if(jbor.eq.1.or.jbor.eq.2.or.jbor.eq.4) kbor = jbor
      if(kbor.gt.0) go to 100
c                      Normative salt designation and printing salt norm
  660 continue
      call convt(minmax,1,2,ss,dxc,0)
      mp(1) = 0
      do 670 i=1,minmax
      s(mm(i)) = ss(i)
      if(s(mm(i)).eq.0.0) mp(1) = 1
  670 continue
c                                                 Simple salt abundances
      i = mr(7)
      s(i) = 0.5*s(30)
      s(i+1) = 0.5*(s(28)+s(29))
      s(i+2) = (2.0*s(26))+s(27)+s(28)
      s(i+3) = s(25)+s(26)
      s(i+4) = s(11)+s(15)+s(16)+(2.0*s(17))
      s(i+5) = s(12)+s(17)+s(18)+s(19)
      s(i+6) = s(14)+s(16)+s(17)+s(19)+(1.5*s(20))
      s(i+7) = s(13)+s(15)+s(18)+(0.5*s(20))
      s(i+8) = s(6)
      s(i+9) = s(4)+s(5)
      s(i+10) = s(2)+s(3)
      s(i+11) = s(1)+s(2)+s(5)
c                                                         Hydroxyapatite
      if(s(51).gt.0.0) call swap(51,0,56,0,19.,1.,12.,1.,s)
c                                                           Borate salts
      if(kbor.gt.-1) go to 765
      do 760 i=43,46
      k = i + 14
      s(k) = s(i)
      s(i) = 0.0
  760 continue
  765 continue
c                               Sulfate salts if chloride-nitrate absent
```

```
      if(x(5).gt.0.0.or.x(11).gt.0.0) go to 768
      if(konk(3).eq.1) go to 768
      if(s(17).eq.0.0.or.s(20).eq.0.0) go to 767
      q=s(17)
      if(q.gt.s(20)) q = s(20)
      q = q*0.5
      s(18) = s(18) + q
      call swap(17,20,16,19,2.,2.,4.,1.,s)
  767 continue
      if(s(11).gt.0.0.and.s(18).gt.0.0)
     1 call swap(11,18,12,15,1.,1.,1.,1.,s)
      if(s(15).gt.0.0.and.s(20).gt.0.0)
     1 call swap(15,20,13,16,3.,2.,4.,3.,s)
  768 continue
c                                                     Double anion salts
      if(s(4).gt..0.and.s(13).gt..0)call swap(4,13,62,0,1.,2.,1.,1.,s)
      if(s(12).gt..0.and.s(29).gt..0)call swap(12,29,61,0,1.,1.,1.,1.,s)
c                                    Stable bicarbonates from carbonates
      if(s(4).gt.0.0) call swap(4,0,63,0,3.,1.,2.,1.,s)
      if(s(6).gt.0.0) call swap(6,0,64,0,1.,1.,2.,1.,s)
      if(s(9).gt.0.0) call swap(9,0,65,0,1.,1.,2.,1.,s)
c                                       Hydration-dehydration equilibria
      sum = s(25) + s(26)
      if(sum.gt.0.0) go to 770
      if(s(32).gt.0.0) call swap(32,0,67,0,1.,1.,1.,1.,s)
      sum = s(35)
      if(sum.gt.0.0) go to 770
      if(s(31).gt.0.0) call swap(31,0,66,0,1.,1.,1.,1.,s)
      sum = s(27) + s(28) + s(66) + s(67) + s(36) + s(35)
      if(sum.gt.0.0) go to 770
      if(s(12).gt.0.0) call swap(12,0,68,0,1.,1.,1.,1.,s)
      sum = s(61)
      q = s(29) + s(30) + s(33) + s(34)
      if(s(68).gt.0.0.and.q.gt.0.0) sum = 1.0
      if(sum.gt.0.0) go to 770
      if(s(19).gt.0.0) call swap(19,0,69,0,1.,1.,1.,1.,s)
      sum = s(29)+s(30)+s(33)+s(34)+s(63)+s(5)+s(64)+s(65)
      if(sum.gt.0.0) go to 770
      if(s(11).gt.0.0) call swap(11,0,70,0,1.,1.,1.,1.,s)
      if(s(13).gt.0.0) call swap(13,0,71,0,1.,1.,1.,1.,s)
  770 continue
      if(kbor.lt.1.or.ctz(3).eq.0.0) go to 780
      q = cz(14,3)
      cz(14,3) = cz(14,3) * (va(14) / (7.0/12.0))
      ctz(3) = ctz(3) + (cz(14,3) - q)
  780 continue
      call print
      go to 800
  790 continue
      if(kbor.lt.1) go to 800
      kbor = -2
      go to 100
  800 continue
      if(kbor.ne.0) kbor = -1
      jj = 15 - minmax
      go to(830,835,840,845,850,855,860,865,870,875,880,885,890,895)jj
  830 continue
  835 continue
  840 continue
  845 continue
  850 continue
  855 continue
  860 continue
  865 continue
  870 continue
  875 continue
  880 continue
  885 continue
  890 continue
  895 continue
  899 continue
      if(kid2.gt.0) go to 900
      kid2 = -1
      call print
  900 continue
      return
      end
c***********************************************************************
```

```
c***********************************************************************
c                         Subroutine PICK
c***********************************************************************
c
c   Determines if new salt added to assemblage is permitted to coexist
c   with previously assigned salts.
c
      subroutine pick(lc,l,i,ma,mb,k,kk,kv,j,mx)
      dimension k(55),kk(14)
      if(kk(1).gt.0) k(kk(1)) = 0
      kk(1) = 0
      if(l.lt.mx) ma = i + 1
      if(l.lt.mx.and.ma.lt.mb) ma = mb
      n = 0
      j = 0
      if(l.eq.1) go to 200
      lc = lc + 1
      nsum1 = k(4)+k(5)+k(6)+k(7)+k(8)+k(9)+k(10)
      nsum2 = k(13)+k(14)+k(15)+k(16)+k(17)+k(18)+k(19)+k(20)
      nsum3 = k(12)+k(13)+k(14)+k(17)+k(18)+k(19)+k(20)
      nsum4 = k(11)+k(12)+k(15)+k(16)+k(17)+k(18)+k(19)
      nsum5 = k(25)+k(26)+k(27)+k(28)
      nsum6 = k(31)+k(32)+k(39)+k(40)
      if(k(11).eq.0.0) nsum6 = 0
      nsum7 = nsum6+k(1)+k(2)+k(5)+k(25)+k(26)+k(35)+k(43)
  110 continue
      go to (200,200,3,3,5,200,200,200,200,200,11,12,13,14,15,16,17
     a,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38
     b,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55) kv
    3 n = k(1)
      go to 200
    5 n = k(3)
      go to 200
   11 n = nsum1
      go to 200
   12 n = nsum1 + k(1)+k(2)
      go to 200
   13 n = k(6)+k(8)+k(9)+k(10)+k(11)+k(12)
      go to 200
   14 n = k(11)+k(12)+k(13)
      go to 200
   15 n = nsum1 + k(12)+k(14)
      go to 200
   16 n = nsum1 + k(12)+k(13)
      go to 200
   17 n = nsum1 + k(1)+k(2)+k(13)+k(14)
      go to 200
   18 n = nsum1 + k(1)+k(2)+k(14)
      if(k(11).eq.1.and.k(16).eq.1) n = n + 1
      go to 200
   19 n = nsum1 + k(1)+k(2)+k(11)+k(13)+k(15)
      if(k(16).eq.1.and.k(18).eq.1) n = n + 1
      go to 200
   20 n = k(6)+k(8)+k(9)+k(10)+k(11)+k(12)
      if(k(15).eq.1.and.k(17).eq.1) n = n + 1
      go to 200
   21 n = k(4)+k(5)+k(6)+k(8)+k(9)
      go to 200
   22 n = k(6)+k(9)
      go to 200
   23 n = k(4)+k(5)+k(6)
      go to 200
   24 n = k(8) + k(9)
      go to 200
   25 n = nsum1 + nsum2 + k(3)+k(12)+k(21)+k(22)+k(23)+k(24)
      go to 200
   26 n = nsum1 + nsum2 + k(1)+k(3)+k(12)+k(21)+k(22)+k(23)+k(24)
      go to 200
   27 n = nsum1 + nsum2 + k(1)+k(23)+k(25)
      if(k(21).eq.1.and.k(2).eq.1) n = n + 1
      go to 200
   28 n = nsum2 +k(4)+k(5)+k(6)+k(9)+k(23)
      if(k(21).eq.1.and.k(1).eq.1) n = n + 1
      if(k(17).eq.1) n = n - 1
      go to 200
   29 n = k(13)+k(15)+k(18)+k(23)+k(26)+k(27)
      if(k(25).eq.1.and.k(2).eq.1) n = n + 1
      if(k(12).eq.1.and.k(11).eq.1) n = n + 1
```

```
      go to 200
   30 n = k(6)+k(9)+k(14)+k(23)
      if(k(19).eq.1.and.k(16).eq.1) n = n + 1
      go to 200
   31 n = nsum2 + k(4)+k(5)+k(6)+k(8)+k(9)+k(12)+k(23)
      if(k(29).eq.1.and.k(11).eq.1.and.k(3).eq.1) n = n + 1
      go to 200
   32 n = nsum2 + k(4)+k(5)+k(6)+k(9)+k(12)+k(21)+k(23)+k(24)
      if(k(29).eq.1.and.k(11).eq.1.and.k(2).eq.1) n = n + 1
      if(k(11).eq.1.and.k(3).eq.1) n = n + 1
      go to 200
   33 n = k(6)
      go to 200
   34 nsum1 = nsum1 - k(10)
      n = nsum1 + nsum2 + k(12) + k(21) + k(23)
      go to 200
   35 n = nsum1 + nsum2 + k(12)+k(21)+k(22)+k(23)+k(24)+k(31)+k(32)
      if(k(3).eq.1.and.k(29).eq.1) n = n + 1
      go to 200
   36 n = nsum1 + nsum2 + k(1)+k(2)+k(23)+k(25)+k(25)+k(26)+k(29)+k(31)+
     a k(34)
      go to 200
   37 n = k(25)+k(26)+k(27)+k(31)+k(32)+k(34)
      if(k(28).eq.1.and.k(1).eq.1) n = n + 1
      if(k(36).eq.1.and.k(30).eq.1) n = n + 1
      go to 200
   38 n =k(6)+k(9)+k(14)+k(16)+k(17)+k(19)+k(20)+k(23)+k(25)+k(26)+
     a k(27)+k(29)+k(31)+k(32)+k(34)
      if(k(28).eq.1.and.k(2).eq.1) n = n + 1
      if(k(28).eq.1.and.k(1).eq.1) n = n + 1
      go to 200
   39 n = nsum2 + k(4)+k(5)+k(6)+k(8)+k(9)+k(12)+k(32)
      if(k(28).eq.1.and.k(22).eq.1.and.k(1).eq.1) n = n + 1
      go to 200
   40 n = nsum2 + k(4)+k(5)+k(6)+k(9)+k(12)+k(21)+k(23)
      if(k(29).eq.1.and.k(11).eq.1.and.k(3).eq.1) n = n + 1
      go to 200
   41 n = k(6)+k(14)+k(25)+k(26)+k(27)+k(28)+k(29)+k(30)+k(31)+
     a k(32)+k(34)
      go to 200
   42 nsum1 = nsum1 - k(10)
      n = nsum1 + nsum2 +k(12)+k(21)+k(22)+k(23)+k(25)+k(26)+k(31)+k(32)
      go to 200
   43 n = k(4)+k(5)+k(12)+k(13)+k(15)+k(17)+k(18)
      go to 200
   44 n = nsum6 + nsum5 + k(4)+k(5)+k(12)+k(13)+k(20)+k(35)
      go to 200
   45 n = nsum6+k(1)+k(4)+k(5)+k(13)+k(15)+k(16)+k(20)+k(25)+
     a k(26)+k(35)
      go to 200
   46 n = nsum5 + nsum6 + k(11)+k(12)+k(35)+k(36)+k(43)
      if(k(17).eq.1.and.k(15).eq.1) n = n + 1
      go to 200
   47 n = k(4)+k(5)+k(12)+k(17)+k(18)+k(19)+k(36)
      go to 200
   48 n = nsum7+k(4)
      go to 200
   49 n = nsum4+nsum5+k(10)+k(24)+k(34)+k(35)+k(36)+k(43)+k(44)+k(45)
      go to 200
   50 n = nsum4 + nsum5 + k(35) + k(36)
      go to 200
   51 n = k(12)+k(17)+k(18)+k(19)+k(47)+k(48)+k(49)+k(50)
      go to 200
   52 n = nsum7+k(47)+k(48)+k(49)+k(50)
      go to 200
   53 n = nsum4 + nsum5 + k(1)+k(2)+k(3)+k(5)+k(35)+k(36)+
     a k(43)+k(44)+k(45)+k(47)+k(48)
      go to 200
   54 n = k(12)+k(17)+k(18)+k(19)+k(52)
      go to 200
   55 n = nsum7+k(47)
      go to 200
  200 continue
      if(n.gt.0) go to 300
      k(kv) = 1
      kk(l) = kv
      if(l.eq.mx) j = -1
      go to 390
```

```
  300 continue
      j = 1
  390 continue
      return
      end
c***********************************************************************
```

```
c***********************************************************************
c                          Subroutine ARRAY
c***********************************************************************
c
c   IBM software converting a double dimension array to a single
c   dimension array.
c
      subroutine array(mode,i,j,n,m,s,d)
      dimension s(1),d(1)
      ni=n-i
      if(mode-1)100,100,120
  100 ij=i*j+1
      nm=n*j+1
      do 110 k=1,j
      nm=nm-ni
      do 110 l=1,i
      ij=ij-1
      nm=nm-1
      d(nm)=s(ij)
  110 continue
      go to 140
  120 ij=0
      nm=0
      do 130 k=1,j
      do 125 l=1,i
      ij=ij+1
      nm=nm+1
      s(ij)=d(nm)
  125 continue
      nm=nm+ni
  130 continue
  140 return
      end
c***********************************************************************
```

```
c***********************************************************************
c                          Subroutine CONVT
c***********************************************************************
c
c   IBM software for converting between single and douuble precision.
c
      subroutine convt(n,m,mode,s,d,ms)
      dimension s(1),d(1)
      double precision d
      if(ms-1)2,4,6
    2 nm=n*m
      go to 8
    4 nm=((n+1)*n)/2
      go to 8
    6 nm=n
    8 if(mode-1)10,10,20
   10 do 15 l=1,nm
      d(l)=dble(s(l))
   15 continue
      go to 30
   20 do 25 l=1,nm
      s(l)=sngl(d(l))
   25 continue
   30 return
      end
c***********************************************************************
```

```
c***********************************************************************
c                          Subroutine DGELG
c***********************************************************************
c
```

```
c    IBM software for solving simultaneous linear equations.
c
      subroutine dgelg(r,a,m,n,eps,ier)
      dimension a(1),r(1)
      double precision r,a,piv,tb,tol,pivi
      if(m)23,23,1
    1 ier=0
      piv=0.d0
      mm=m*m
      nm=n*m
      do 3 l=1,mm
      tb=dabs(a(l))
      if(tb-piv)3,3,2
    2 piv=tb
      i=l
    3 continue
      tol=eps*piv
      lst=1
      do 17 k=1,m
      if(piv)23,23,4
    4 if(ier)7,5,7
    5 if(piv-tol)6,6,7
    6 ier=k-1
    7 pivi=1.d0/a(i)
      j=(i-1)/m
      i=i-j*m-k
      j=j+1-k
      do 8 l=k,nm,m
      ll=l+i
      tb=pivi*r(ll)
      r(ll)=r(l)
      r(l)=tb
    8 continue
      if(k-m)9,18,18
    9 lend=lst+m-k
      if(j)12,12,10
   10 ii=j*m
      do 11 l=lst,lend
      tb=a(l)
      ll=l+ii
      a(l)=a(ll)
      a(ll)=tb
   11 continue
   12 do 13 l=lst,mm,m
      ll=l+i
      tb=pivi*a(ll)
      a(ll)=a(l)
      a(l)=tb
   13 continue
      a(lst)=j
      piv=0.d0
      lst=lst+1
      j=0
      do 16 ii=lst,lend
      pivi=-a(ii)
      ist=ii+m
      j=j+1
      do 15 l=ist,mm,m
      ll=l-j
      a(l)=a(l)+pivi*a(ll)
      tb=dabs(a(l))
      if(tb-piv)15,15,14
   14 piv=tb
      i=l
   15 continue
      do 16 l=k,nm,m
      ll=l+j
      r(ll)=r(ll)+pivi*r(l)
   16 continue
      lst=lst+m
   17 continue
   18 if(m-1)23,22,19
   19 ist=mm+m
      lst=m+1
      do 21 i=2,m
      ii=lst-i
      ist=ist-lst
      l=ist-m
```

```
      l=a(1)+0.5d0
      do 21 j=ii,nm,m
      tb=r(j)
      ll=j
      do 20 k=ist,mm,m
      ll=ll+1
      tb=tb-a(k)*r(ll)
   20 continue
      k=j+1
      r(j)=r(k)
      r(k)=tb
   21 continue
   22 return
   23 ier=-1
      go to 22
      end
c***********************************************************************
```

```
c***********************************************************************
c                               Subroutine SWAP
c***********************************************************************
c
c   Solves equation for forming double-anion salts, and salts with
c   correct hydration state.
c
      subroutine swap(m1,m2,n1,n2,r1,r2,p1,p2,sw)
      dimension m(2),n(2),r(2),p(2),sw(99)
      m(1) = m1
      m(2) = m2
      n(1) = n1
      n(2) = n2
      r(1) = r1
      r(2) = r2
      p(1) = p1
      p(2) = p2
      q=1.0e+10
      do 10 i=1,2
      if(m(i).eq.0) go to 20
      qq = sw(m(i)) / r(i)
      if(q.gt.qq) k = i
      if(q.gt.qq) q = qq
   10 continue
   20 continue
      do 50 i=1,2
      if(m(i).gt.0) sw(m(i)) = sw(m(i)) - (q*r(i))
      if(k.eq.i) sw(m(i)) = 0.0
      if(n(i).gt.0) sw(n(i)) = sw(n(i)) + (q*p(i))
   50 continue
      return
      end
c***********************************************************************
```

```
c***********************************************************************
c                               Subroutine PRINT
c***********************************************************************
c
c   Formats output to user specification and prints salt norm.
c
      subroutine print
      character*5 iput
      character*5 nicht,joo,day
      character*6 nsim,ksim
      character*30 kpa,kpb,kpc,kpd,kap,kbp,kcp
      character*9 jo,koodle,noodle,moodle,ipux,ipuz
      character*10 kun,kku,nrat
      character*15 lmi
      character*19 ko,start
      character*20 lmf
      character*42 lbor
      character*31 nsf
      dimension is(99),ia(99),ip(99),swa(99),swh(99),sout(99,12),ko(21),
     a kq(4),kz(2),kku(9),kun(7),
```

```
     b li(25),jo(12),joo(2),oo(8),day(2),rat(21),nrat(21),kr(21),kc(21),
     c souts(12),iput(8),ndel(10),sa(99),ju(8),jv(8),lbor(5),jbor(4),
     d nsim(13),ksim(20),ipux(9),ipuz(4),ig(12),js(12),ssw(12),ssm(12)
      character*80 nbatch
      character*40 ndes
      character*20 mf
      character*15 nmin
      character*13 nsimp,lout,lloc
      character*10 nfile,nnum
      character*5 ncom
      common ncom(25),atw(25),nv(25),v(25),va(25),chg,kbor,nitro,np,kid,
     a ncfn,nnox,nc,cz(25,14),nnax,lout,kbri,kfile,s(99),kred,npage,kxt,
     c isalt(99),lunit,konf,nix(25),nnix,x(25),xo(25),c(25),lloc,nbatch,
     d kend,to(25),kid2,kfirst,kpage,ndes,nnum,nuts,nmin(99),kbank,kidl,
     e nfile,muts,mf(99),lc(99,6),lz(99,6),lh(99),la(99),z(99,6),ph,den,
     f must(10),nsimp,nu(10),naly(99),kid3,mp(9),mr(9),ctz(14),nax(25)
      data lmf/'                    '/
      data lmi/'               '/
      data nsim/'Na2Cl2','K2Cl2 ','MgCl2 ','CaCl2 ','CaSO4 ',
     a          'MgSO4 ','K2SO4 ','Na2SO4','K2CO3 ','Na2CO3',
     b          'MgCO3 ','CaCO3 ','      '/
      data noodle/'     -    '/
      data koodle/'     -    '/
      data moodle/'          '/
      data nicht/' nd  '/
      data li/2,1,13,12,9,3,4,10,15,5,16,17,11,18,8,6,14,7,7*19/
      data ipux/'  mol/kg ','  %(mol) ','   %(wt) ',' %(an-wt)',
     a'   mol/l ', '   eq/kg ','    eq/l ','   molal ','eq/kg-H2O'/
      data kun/'  moles   ','    mg    ',' mg (anhy)',
     a         '   mole   ','  weight  ',' wt.(anhy)','   equiv. '/
      data kpa/'     per kilogram of water    '/
      data kpb/'   per kilogram of solution   '/
      data kpc/'    per liter of solution     '/
      data kpd/'  normative salts - percent   '/
      data iput/'molal','mg/kg','meq/l',' mg/l',' mM/l','g/kgW',
     a' M/kg','     '/
      data kc/1,2,3,4,5,10,18,19,20,14,11,17,7,6,16,15,12,8,9,13,21/
      data ig/3,2,1,9,10,11,12,5,6,8,7,4/
      data nrat/'      Ca/Mg','       K/Na','Mg+Ca/Na+K',' alk./hal.',
     a'    HCO3/Cl','      Ca/Cl','      Mg/Cl','      Na/Cl','       K/Cl',
     a          '     SO4/Cl','     PO4/Cl','      Li/Cl','     NH4/Cl',
     a          '     NO3/Cl','      Ba/Cl','      Sr/Cl','       B/Cl',
     a          '       F/Cl','      Br/Cl','       I/Cl','           '/
      data lbor/'Inyoite - Ca(1.79)B(6.14)O(11).13H2O    ',
     a          'Ulexite - Na(0.98)Ca(0.98)B(5.02)O(9).8H2O',
     b          'Indirite - Mg(1.79)B(6.14)O(11).15H2O   ',
     c          'Borax - Na(2.28)B(3.91)O(7).10H2O       ',
     d          '                                        '/
      call cdate(jmonth,jday,jyear)
      if(mp(1).eq.0) go to 150
      nqq = 0
      do 120 i=1,np
      if(kid2.eq.0) ia(i) = 0
      if(kid2.gt.0) ia(i) = isalt(i)
      isalt(i) = 0
      if(s(i).gt.0.0) isalt(i) = 1
      if(ia(i).ne.isalt(i)) nqq = 1
  120 continue
      if(nqq.eq.0) go to 799
  150 continue
      kid2 = kid2 + 1
c
c                                                        Lines per page
c
      lunit = nu(10)
      ntime = 0
      kp = 0
      if(kpage.eq.1) kp = 1
      if(kpage.eq.2) lunit = nu(4)
      if(kpage.eq.2.and.kfile.eq.2) lunit = nu(5)
  200 continue
      lmax = 66
      if(lunit.eq.nu(5).and.npage.eq.0) lmax = 62
      if(lunit.eq.nu(4)) lmax = 60
      note = 1
      if(to(8).gt.0.0) note = note + 1
      if(mr(9).eq.1.and.kid2.ne.0) note = note + 1
      if(den.eq.0.0) note = note + 1
```

```
      if(muts.eq.1.or.muts.eq.3.or.muts.eq.4) note = note + 1
      if(kbri.ne.0.and.kid2.ne.0) note = note + 1
      if(kbor.lt.0.and.kid2.ne.0) note = note + 1
      if(s(56).gt.0.0.and.kid2.ne.0) note = note + 1
      if(mp(2).ne.0) note = note + 1
      if(nnax.ne.0) note = note + 1
      if(mp(3).ne.0) note = note + 1
      j = 0
      do 205 i=57,60
      if(s(i).gt.0.0) j = j + 1
  205 continue
      if(j.gt.2.and.kid2.ne.0) note = note + 1
c
c                                                   Data bank print-out
c
      if(kbank.eq.0) go to 300
      if(kp.ne.1) go to 240
      do 220 i=1,nc
      write(lunit,901) i,ncom(i),atw(i),nv(i)
  220 continue
      do 230 i=1,mr(8)
      write(lunit,902) i,nmin(i),mf(i),(lc(i,k),lz(i,k),k=1,lh(i))
  230 continue
      go to 300
  240 continue
      npage = npage + 1
      numb  = 5
      write(lunit,905)
      do 250    i=1,nc
      write(lunit,907) i,ncom(i),atw(i),nv(i),i,
     a    nmin(i),mf(i),(lc(i,k),lz(i,k),k=1,lh(i))
      numb = numb + 1
  250 continue
      llmax = lmax - 3
      nnc = nc + 1
      do 270    i=nnc,mr(8)
      write(lunit,908) i,nmin(i),mf(i),(lc(i,k),lz(i,k),k=1,lh(i))
      if(lunit.eq.nu(4)) go to 270
      numb = numb + 1
      if(numb.ne.llmax) go to 270
      write(lunit,906)
      numb = 3
  270 continue
      if(lunit.eq.nu(4)) go to 300
      it = numb + 1
      do 280 i=it,lmax
      write(lunit,864)
  280 continue
  300 continue
c
c                                                 Salt molecular weights
c
      if(ntime.ne.0) go to 600
      ntime = 1
      if(kid2.eq.0) go to 400
      atw(5) = 35.453
      if(kbri.eq.0) go to 320
      sum = c(5) + c(16) + c(17)
      ratbr = 100.0*(c(16)/sum)
      rati = 100.0*(c(17)/sum)
      ratcl = 100.0*(c(5)/sum)
      atw(5) = ((ratbr*atw(16))+(rati*atw(17))+(ratcl*atw(5)))/100.0
  320 continue
      nsal = 0
      tswh = 0.0
      tswa = 0.0
      do 360 i=1,mr(8)
      sa(i) = 0.0
      swh(i) = 0.0
      swa(i) = 0.0
      if(s(i).eq.0.0) go to 360
      if(i.le.np) nsal = nsal + 1
      do 350  k=1,lh(i)
      swh(i) = swh(i) + (z(i,k) * atw(lc(i,k)))
      if(lc(i,k).eq.19) go to 350
      swa(i) = swa(i) + (z(i,k) * atw(lc(i,k)))
  350 continue
  360 continue
```

```
  400 continue
c
c                                         Calculation of mole ratios
c
      do 410 i=1,21
      rat(i) = 0.0
  410 continue
      if(to(1).eq.0.0.or.to(2).eq.0.0) go to 430
      rat(1) = to(1) / to(2)
  430 continue
      if(to(3).eq.0.0.or.to(4).eq.0.0) go to 440
      rat(2) = to(4) / to(3)
  440 continue
      if(to(1).eq.0.0.and.to(2).eq.0.0) go to 450
      if(to(3).eq.0.0.and.to(4).eq.0.0) go to 450
      rat(3) = (to(1) + to(2)) / (to(3) + to(4))
  450 continue
      q = to(3) + to(4)
      qq = to(5) + to(16) + to(17)
      if(q.eq.0.0.or.qq.eq.0.0) go to 452
      rat(4) = q/qq
  452 continue
      q = to(18) + (2.0 * to(8))
      if(to(5).eq.0.0) go to 470
      if(q.eq.0.0) go to 455
      rat(5) = q/to(5)
  455 continue
      q = to(5)
      if(q.eq.0) go to 470
      ki = 5
      do 460 i=1,nc
      if(i.eq.5.or.i.eq.8.or.i.eq.18) go to 460
      if(i.eq.19.or.i.eq.20.or.i.eq.21) go to 460
      ki = ki + 1
      if(to(i).eq.0.0) go to 460
      rat(ki) = to(i) / q
  460 continue
  470 continue
      ki = 0
      do 480 i=1,21
      if(rat(kc(i)).eq.0.0) go to 480
      ki = ki + 1
      kr(ki) = kc(i)
  480 continue
      ki = ki + 1
      do 485 i=ki,21
      kr(i) = 21
  485 continue
      do 490 i=1,21
      if(rat(kr(i)).gt.0.0) write(start,818) nrat(kr(i)),rat(kr(i))
      if(rat(kr(i)).eq.0.0) write(start,819) nrat(21)
      read(start,820) ko(i)
  490 continue
c
c                              Recasting solutes and salts into various units
c
      rata = 0.0
      ratb = 0.0
      ratc = 0.0
      if(kxt.eq.0) rata = 1.0
      if(kxt.eq.1) ratc = 1.0
      nsol = 0
      do 520 i=1,nc
      do 500 j=8,14
      cz(i,j) = 0.0
      if(i.eq.1) ctz(j) = 0.0
  500 continue
      if(c(i).gt.0.0.or.to(i).gt.0.0) nsol = nsol + 1
      if(c(i).eq.0.0) go to 520
      if(kxt.eq.1) go to 510
      cz(i,8) = c(i)
      cz(i,9) = c(i) * atw(i) * 1000.0
      ctz(8) = ctz(8) + cz(i,8)
      ctz(9) = ctz(9) + cz(i,9)
      go to 520
  510 continue
      cz(i,10) = c(i) * va(i) * 1000.0
      cz(i,11) = c(i) * atw(i) * 1000.0
```

```
    cz(i,12) = c(i) * 1000.0
    ctz(10) = ctz(10) + cz(i,10)
    ctz(11) = ctz(11) + cz(i,11)
    ctz(12) = ctz(12) + cz(i,12)
520 continue
    if(kxt.eq.1) go to 530
    ratb = 1000.0 / ((ctz(9)/1000.0) + 1000.0)
    ctz(9) = 0.0
    ratc = ratb * den
    do 525 i=1,nc
    if(cz(i,9).eq.0.0) go to 525
    cz(i,9) = cz(i,9) * ratb
    cz(i,11) = cz(i,9) * den
    cz(i,12) = cz(i,11) / atw(i)
    cz(i,10) = (cz(i,11) * va(i)) / atw(i)
    ctz(9) = ctz(9) + cz(i,9)
    ctz(10) = ctz(10) + cz(i,10)
    ctz(11) = ctz(11) + cz(i,11)
    ctz(12) = ctz(12) + cz(i,12)
525 continue
    go to 540
530 continue
    if(den.eq.0.0) go to 540
    ratb = ratc / den
    rata = 1000.0 / ((1000.0*den) - (ctz(11)/1000.0))
    do 535 i=1,nc
    if(cz(i,11).eq.0.0) go to 535
    cz(i,8) = (rata * c(i))
    cz(i,9) = ratb * cz(i,11)
    ctz(8) = ctz(8) + cz(i,8)
    ctz(9) = ctz(9) + cz(i,9)
535 continue
540 continue
    if(ctz(1).eq.0.0) go to 543
    do 542 i=1,nc
    if(cz(i,8).eq.0.0) go to 542
    cz(i,13) = cz(i,8)*atw(i)
    cz(i,14) = cz(i,9)/(1000.0*atw(i))
    ctz(13) = ctz(13) + cz(i,13)
    ctz(14) = ctz(14) + cz(i,14)
542 continue
543 continue
    do 550 k=1,12
    souts(k) = 0.0
    js(k)=0
    ssw(k)=0.0
    ssm(k)=0.0
    do 545 i=1,99
    sout(i,k) = 0.0
    if(k.eq.1) ip(i) = 99
545 continue
550 continue
    if(kid2.eq.0) go to 600
    jout = 0
    if(nuts.eq.1) jout = 1
    if(kxt.eq.1) jout = 2
    if(kred.eq.0) go to 554
    if(kred.ne.1) go to 551
    if(kxt.eq.0) jout = 1
    if(den.gt.0.0) jout = 1
551 continue
    if(kred.ne.2) go to 552
    if(jout.eq.1) jout = 0
    if(den.gt.0.0) jout = 0
552 continue
    if(kred.ne.3) go to 554
    if(den.gt.0.0) jout = 2
554 continue
    do 565 i=1,np
    if(s(i).eq.0.0) go to 565
    if(jout.eq.0) sout(i,1) = s(i)*ratb
    if(jout.eq.1) sout(i,1) = s(i)*rata
    if(jout.eq.2) sout(i,1) = s(i)*ratc
    sout(i,2) = sout(i,1)*swh(i)*1000.0
    sout(i,3) = sout(i,1)*swa(i)*1000.0
    if(mr(9).eq.0) go to 560
    q = 0.0
    do 555 j=1,la(i)
```

```
      if(v(lc(i,j)).gt.0.0) q=q+(v(lc(i,j))*z(i,j))
  555 continue
      sout(i,1) = sout(i,1)*q
  560 continue
      souts(1) = souts(1) + sout(i,1)
      souts(2) = souts(2) + sout(i,2)
      souts(3) = souts(3) + sout(i,3)
  565 continue
      do 575 i=1,np
      if(s(i).eq.0.0) go to 575
      do 570 k=4,6
      kk = k-3
      sout(i,k) = 100.0*(sout(i,kk)/souts(kk))
      souts(k) = souts(k) + sout(i,k)
  570 continue
      sa(i) = sout(i,2)
  575 continue
      k = 0
      sum7 = 0.0
      sum8 = 0.0
      do 580 i=mr(7),mr(8)
      if(s(i).eq.0.0) go to 580
      j = i-(mr(7) - 1)
      k = k + 1
      js(k)=j
      ksim(k) = nsim(j)
      sout(k,7) = s(i)
      sout(k,8) = sout(k,7)*swh(i)*1000.0
      sum7 = sum7 + sout(k,7)
      sum8 = sum8 + sout(k,8)
  580 continue
      do 581 i=1,k
      sout(i,7) = 100.0*(sout(i,7)/sum7)
      sout(i,8) = 100.0*(sout(i,8)/sum8)
      souts(7) = souts(7) + sout(i,7)
      souts(8) = souts(8) + sout(i,8)
      ssw(js(i))=sout(i,8)
      ssm(js(i))=sout(i,7)
  581 continue
      if(mp(5).eq.0) go to 584
      junk=2
      if(nuts.gt.2) junk=1
      if(junk.eq.1) trash=ctz(4)
      if(junk.eq.2) trash=ctz(2)
      if(kid.eq.0) write(nu(7),993) ndes,nnum,trash,junk
      if(kid.eq.1) write(nu(7),996) nbatch,trash,junk
      j2=0
      do 583 i=1,3
      j1=j2+1
      j2=j1+3
      write(nu(7),994) (ssw(ig(j)),ssm(ig(j)),j=j1,j2)
  583 continue
  584 continue
      lsim = k
      linmax = nsal
      if(lsim.gt.nsal) linmax = lsim
      do 586 i=1,linmax
      if(i.gt.nsal) ip(i) = 99
      if(i.gt.lsim) ksim(i) = nsim(13)
  586 continue
      nmin(99) = lmi
      mf(99) = lmf
  588 continue
c
c                                  Arranging out-put in decreasing order
c
      k = 0
  590 continue
      k = k + 1
      q = -1.0
      do 595    i=1,np
      if(sa(i).le.q) go to 595
      q = sa(i)
      ip(k) = i
  595 continue
      if(sa(ip(k)).eq.0.0) go to 600
      sa(ip(k)) = -1.0
      go to 590
```

```
  600 continue
      ip(k) = 99
c
c                                    Printing solution composition
c
      if(kp.eq.1) go to 630
      if(kid2.eq.0) nsal = -5
      ltot = 26 + linmax + nsol + note
      ldif = lmax - ltot
      k = 0
      if(ldif.le.0) go to 620
      if(lunit.eq.nu(4)) write(lunit,807)
      if(lunit.eq.nu(4)) ldif = ldif - 1
      if(ldif.lt.1) go to 625
      do 610 i=1,ldif,2
      if(i.eq.1) go to 610
      k = k + 1
      write(lunit,864)
  610 continue
      ldif = ldif - k
      go to 625
  620 continue
      if(lunit.eq.nu(10).or.lunit.eq.nu(5)) go to 625
      write(lunit,810) nbatch
      go to 630
  625 continue
      write(lunit,811) nbatch
  630 continue
      iput(8) = iput(nuts)
      if(kid.eq.0.and.kp.ne.1) write(lunit,812) ndes,nnum
      if(kp.eq.1) write(lunit,911) nbatch
      if(kid.eq.0.and.kp.eq.1) write(lunit,912) ndes,nnum
      if(kp.ne.1) write(lunit,813)
      if(kp.eq.1) write(lunit,913)
      write(start,804) ph
      read(start,805) joo(1)
      write(start,806) den
      read(start,805) joo(2)
      if(ph.eq.20.0) joo(1) = nicht
      if(den.eq.0.0) joo(2) = nicht
      if(kp.ne.1.and.ldif.ge.0) write(lunit,864)
      if(kp.ne.1.and.ldif.lt.0) ldif = ldif + 1
      if(kp.ne.1) write(lunit,816) (joo(i),i=1,2)
      if(kp.ne.1.and.ldif.ge.-2) write(lunit,864)
      if(kp.ne.1.and.ldif.lt.-2) ldif = ldif + 1
      kkp = 4
      if(kp.eq.1) kkp = 2
      kkq = kkp + kkp
      jv(1) = 1
      if(kp.eq.1) go to 640
      if(muts.eq.5.or.muts.eq.6) jv(1) = 7
      if(muts.eq.8) jv(1) = 2
      jv(2) = 6
      if(muts.eq.2.or.muts.gt.6) jv(2) = 3
      if(muts.eq.5.or.muts.eq.6) jv(2) = 2
      jv(3) = 5
      if(muts.eq.1) jv(3) = 7
      if(muts.eq.3.or.muts.eq.5) jv(3) = 3
      jv(4) = 4
      if(muts.eq.1) jv(4) = 2
      go to 645
  640 continue
      if(kp.ne.1) go to 645
      jv(1) = 7
      if(jout.eq.1) jv(1) = 1
      if(jout.eq.2) jv(1) = 5
      jv(2) = nuts
      if(jv(1).ne.jv(2)) go to 645
      if(jout.eq.1) jv(2) = 6
      if(jout.eq.2) jv(2) = 4
  645 continue
      do 650 i=1,kkp
      k = i + kkp
      jv(k) = jv(i)
      ju(i) = jv(i)
      ju(k) = ju(i) + 7
  650 continue
  660 continue
```

```
      if(kp.ne.1) write(lunit,821) iput(8)
      if(kp.eq.1) write(lunit,921) iput(8),(joo(i),i=1,2)
      ki = 1
      if(kp.ne.1) write(lunit,822) (iput(jv(i)),i=1,4),
     a ko(ki),(iput(jv(i)),i=5,8)
      if(kp.eq.1) write(lunit,925)
      if(kp.eq.1) write(lunit,926)
      if(kp.eq.1)write(lunit,927)(iput(jv(i)),i=1,4),ko(ki)
      ki = ki + 1
      if(kp.eq.1) write(lunit,928) ko(ki)
      if(kp.ne.1.and.ldif.ge.-2) write(lunit,823) ko(ki)
      if(kp.ne.1.and.ldif.ge.-2) ki = ki + 1
      if(kp.ne.1.and.ldif.lt.-2) ldif = ldif + 1
      if(kp.eq.1) ki = ki + 1
      ki = ki - 1
      do 685 i=1,nc
      if(to(li(i)).eq.0.0.and.c(li(i)).eq.0.0) go to 685
      do 680    k=1,kkq
      write(start,801) cz(li(i),ju(k))
      read(start,802) jo(k)
      if(cz(li(i),ju(k)).eq.0.0) jo(k) = koodle
  680 continue
      if(ki.lt.21) ki = ki +1
      if(kp.ne.1) write(lunit,831) ncom(li(i)),(jo(k),k=1,4),ko(ki),
     a ncom(li(i)),(jo(k),k=5,8)
      if(kp.eq.1) write(lunit,931) ncom(li(i)),(jo(k),k=1,4),ko(ki)
  685 continue
      if(ki.lt.21) ki = ki + 1
      if(kp.ne.1) write(lunit,835) ko(ki)
      if(kp.eq.1) write(lunit,935) ko(ki)
      do 690 k=1,kkq
      write(start,801) ctz(ju(k))
      read(start,802) jo(k)
      if(ctz(ju(k)).eq.0.0) jo(k) = koodle
  690 continue
      if(ki.lt.21) ki = ki + 1
      cbo = va(14)
      if(kp.ne.1) write(lunit,836) (jo(k),k=1,4),ko(ki),(jo(k),k=5,8)
      if(kp.eq.1) write(lunit,936) (jo(k),k=1,4),ko(ki)
      if(kp.ne.1.and.ldif.ge.-2) write(lunit,864)
      if(kp.ne.1.and.ldif.lt.-2) ldif = ldif + 1
      if(kbor.eq.0.or.kp.eq.1) write(lunit,840) chg
      if(kp.ne.1.and.kbor.ne.0) write(lunit,845) chg,cbo
      if(kp.eq.1.and.kbor.ne.0) write(lunit,945) cbo
c
c                                                  Printing salt norm
c
      if(kp.eq.1) write(lunit,864)
      if(jout.eq.0) kap = kpb
      if(jout.eq.1) kap = kpa
      if(jout.eq.2) kap = kpc
      kbp = kpd
      do 710 i=1,8
      ii = i
      if(i.gt.6) ii = i-3
      kku(i) = kun(ii)
  710 continue
      if(mr(9).eq.1) kku(1) = kun(7)
      if(mr(9).eq.1) kku(4) = kun(7)
      if(kp.ne.1) go to 720
      do 715 i=1,4
      ipuz(i) = ipux(i)
  715 continue
      if(jout.eq.1) ipuz(1) = ipux(8)
      if(jout.eq.2) ipuz(1) = ipux(5)
      if(mr(9).eq.0) go to 720
      if(jout.eq.0) ipuz(1) = ipux(6)
      if(jout.eq.1) ipuz(1) = ipux(9)
      if(jout.eq.2) ipuz(1) = ipux(7)
  720 continue
      if(kp.ne.1.and.ldif.ge.-2) write(lunit,864)
      if(kp.ne.1.and.ldif.lt.-2) ldif = ldif + 1
      if(kid2.eq.0) go to 750
      if(kp.ne.1) write(lunit,853)
      if(kp.ne.1) write(lunit,861) kap,kbp
      if(kp.ne.1) write(lunit,862)
      if(kp.ne.1) write(lunit,863) (kku(i),i=1,8)
      if(kp.eq.1) write(lunit,953)
```

```
      if(kp.eq.1) write(lunit,950) (ipuz(i),i=1,4)
      if(kp.eq.1) write(lunit,864)
      if(kp.ne.1.and.ldif.ge.-1) write(lunit,864)
      if(kp.ne.1.and.ldif.lt.-1) ldif = ldif + 1
      kk = 8
      if(kp.eq.1) kk = 6
      ninmax = linmax
      if(kp.eq.1) ninmax = nsal
      do 740 i=1,ninmax
      do 735 k=1,kk
      ii = ip(i)
      if(k.gt.6) ii=i
      if(k.lt.4) write(start,801) sout(ii,k)
      if(k.gt.3) write(start,803) sout(ii,k)
      read(start,802) jo(k)
      if(sout(ii,k).eq.0.0) jo(k) = moodle
  735 continue
      if(kp.ne.1) write(lunit,870)nmin(ip(i)),mf(ip(i)),
     a (jo(k),k=1,6),ksim(i),(jo(k),k=7,8)
      if(kp.eq.1) write(lunit,970)nmin(ip(i)),mf(ip(i)),
     a jo(1),(jo(k),k=4,6)
  740 continue
      do 745 k=1,kk
      if(k.lt.4) write(start,801) souts(k)
      if(k.gt.3) write(start,803) souts(k)
      read(start,802) jo(k)
  745 continue
      if(kp.ne.1) write(lunit,875)
      if(kp.eq.1) write(lunit,975)
      if(kp.ne.1) write(lunit,876) (jo(k),k=1,8)
      if(kp.eq.1) write(lunit,976) jo(1),(jo(k),k=4,6)
      if(kp.ne.1) go to 750
      write(lunit,864)
      write(lunit,977)
      do 747 i=1,lsim
      do 746 k=7,8
      write(start,803) sout(i,k)
      read(start,802) jo(k)
  746 continue
      write(lunit,978) ksim(i),jo(7),jo(8)
  747 continue
      write(lunit,981)
      do 748 k=7,8
      write(start,803)souts(k)
      read(start,802)jo(k)
  748 continue
      write(lunit,979)jo(7),jo(8)
  750 continue
      if(kid2.ne.0) go to 755
      if(kp.ne.1) write(lunit,895)
      if(kp.eq.1) write(lunit,995)
  755 continue
      if(kp.ne.1) write(lunit,813)
      if(kp.eq.1) write(lunit,913)
c                                                   Printing footnotes
      knote = 1
      if(kp.ne.1.and.to(8).gt.0.0) write(lunit,881) knote
      if(kp.ne.1.and.to(8).eq.0.0) write(lunit,891) knote
      if(kp.eq.1) write(lunit,990) knote
      if(kp.eq.1.and.to(8).gt.0.0) write(lunit,991)
      if(kp.eq.1) write(lunit,992)
      knote = knote + 1
      if(kp.eq.1) go to 760
      if(den.eq.0.0.and.kxt.eq.0) write(lunit,882) knote
      if(den.eq.0.0.and.kxt.eq.1) write(lunit,883) knote
      if(den.eq.0.0) knote = knote + 1
  760 continue
      i = 0
      if(muts.eq.1.or.muts.eq.3.or.muts.eq.4) i = 1
      if(i.eq.1) write(lunit,879) knote
      if(i.eq.1) knote = knote + 1
      if(mp(2).eq.1) write(lunit,884) knote
      if(mp(2).eq.1) knote = knote + 1
      if(mp(2).eq.2) write(lunit,885) knote
      if(mp(2).eq.2) knote = knote + 1
      if(mp(3).ne.0) write(lunit,886) knote
      if(mp(3).ne.0) knote = knote + 1
      if(nnax.eq.0) go to 775
```

```
      do 765 i=1,10
      ndel(i) = nc + 1
  765 continue
      kk = 0
      do 770 i=1,nc
      if(nax(i).eq.0) go to 770
      kk = kk + 1
      ndel(kk) = i
  770 continue
      if(kk.eq.0) go to 775
      write(lunit,887) knote,(ncom(ndel(i)),i=1,10)
      knote = knote + 1
  775 continue
      if(kid2.eq.0) go to 780
      if(mr(9).eq.1) write(lunit,892) knote
      if(mr(9).eq.1) knote = knote + 1
      if(kbri.eq.0) go to 777
      if(ratbr.gt.9.9.or.rati.gt.9.9)write(lunit,8888)knote,ratbr,rati
      if(ratbr.le.9.9.and.rati.le.9.9)write(lunit,888)knote,ratbr,rati
      knote = knote + 1
  777 continue
      if(s(56).gt.0.0) write(lunit,890) knote
      if(s(56).gt.0.0) knote = knote + 1
      if(kbor.ge.0) go to 780
      j = 0
      do 778 i=1,4
      jbor(i) = 5
      k = i + 56
      if(s(k).eq.0.0) go to 778
      j = j + 1
      jbor(j) = i
  778 continue
      if(jbor(1).eq.5) go to 780
      if(kp.eq.1) go to 779
      write(lunit,889)knote,lbor(jbor(1)),lbor(jbor(2))
      if(j.gt.2) write(lunit,8891)lbor(jbor(3))
      knote = knote + 1
      if(j.gt.2) knote = knote + 1
      go to 780
  779 continue
      write(lunit,989)knote,lbor(jbor(1))
      if(j.gt.1)write(lunit,9891)lbor(jbor(2))
      if(j.gt.2)write(lunit,9891)lbor(jbor(3))
  780 continue
       if(mp(5).eq.0) write(nsf,947)
       if(mp(5).eq.1) write(nsf,948) nfile
      ldif = ldif + (note - (knote - 1))
      if(kp.ne.1.and.ldif.ge.0) write(lunit,864)
      if(kp.ne.1.and.ldif.lt.0) ldif = ldif + 1
      if(kp.ne.1) write(lunit,880) kidl,nfile,nsf,jmonth,jday,jyear
      if(kp.eq.1) write(lunit,980) kidl,nfile,nsf,jmonth,jday,jyear
      if(kp.eq.1) write(lunit,864)
      if(kp.eq.1) write(lunit,864)
      if(kp.eq.1) go to 790
      if(lunit.eq.nu(4)) go to 790
      if(ldif.lt.1) go to 790
      do 785 i=1,ldif
      write(lunit,864)
  785 continue
  790 continue
      if(kfile.eq.0.or.lunit.eq.nu(5)) go to 795
      if(lunit.eq.nu(4).and.kfile.eq.1) go to 795
      if(lunit.eq.nu(4)) lunit = nu(5)
      if(lunit.eq.nu(10).and.kfile.ne.2) lunit = nu(4)
      if(lunit.eq.nu(10)) lunit = nu(5)
      kp = 0
      go to 200
  795 continue
      npage = npage + 1
      kbank = 0
  799 continue
      return
  801 format(1pe9.3)
  802 format(a9)
  803 format(0pf9.5)
  804 format(0pf5.2)
  805 format(a5)
  806 format(0pf5.3)
```

```
 807 format('1',1x)
 808 format(a9)
 810 format('1',a80)
 811 format(' ',a80)
 812 format(' ',a40,81x,a10)
 813 format(' ',131('-'))
 816 format(' ','Solution properties:',10x,'ph = ',a5,10x,
    a 'density = ',a5)
 818 format(a10,1x,1pe8.2)
 819 format(a10,9x)
 820 format(a19)
 821 format(' ',4x,'Water composition (analytical units: ',a5,')',15x,
    a'Mole ratios',8x,
    a'Concentrations adjusted to achieve charge balance',/,2x,
    b 49('-'),31x,49('-'))
 822 format(' ',8x,4(2x,a5,4x),3x,a19,14x,4(2x,a5,4x))
 823 format(' ',55x,a19)
 831 format(' ',1x,a5,4(2x,a9),5x,a19,7x,a5,4(2x,a9))
 835 format(' ',6x,4(2x,9('-')),5x,a19,12x,4(2x,9('-')))
 836 format(' ',1x,'Total',4(2x,a9),5x,a19,7x,'Total',4(2x,a9))
 840 format(' ',5x,'Charge balance:  sum[+]/sum[-] = ',f6.4)
 845 format(' ',5x,'Charge balance:  sum[+]/sum[-] = ',f6.4,
    127x,'Note: borate charge of -',f5.3,' per boron.')
 864 format(' ',1x)
 853 format(' ','Normative salt assemblage',77x,'Simple salts',/,1x,
    a 25('-'),77x,12('-'))
 861 format(' ',36x,a30,1x,a30,15x,6x,'percent')
 862 format(' ',36x,29('-'),2x,29('-'),16x,19('-'))
 863 format(' ',34x,2(1x,3a10),15x,2a10)
 870 format(' ',a15,1x,a20,3(a9,1x),1x,3(a9,1x),8x,a6,2(1x,a9))
 875 format(' ',36x,3(9('-'),1x),1x,3(9('-'),1x),14x,2(1x,9('-')))
 876 format(' ',25x,'Total',6x,3(a9,1x),1x,3(a9,1x),14x,2(1x,a9))
 879 format(' ',7x,i1,'. g/kgW = grams per kilogram water.')
 880 format(' ','Sample ',i2,' in file: ',a10,29x,a31,30x,i2,'-',
    -i2.2,'-',i4)
 881 format(' ','NOTES: ',i1,'. Solute mole ratios calculated from '
    a ,'initial analytical data; HCO3 includes CO3 via '
    b ,'CO3 + CO2 + H2O = 2HCO3;',/,11x,'alkali/halide ratio ',
    c'excludes lithium and fluoride.')
 891 format(' ','NOTES: ',i1,'. Solute mole ratios calculated from '
    a,'initial analytical data; alkali/halide ratio excludes lithium ',
    b'and fluoride.')
 882 format(' ',7x,i1,'. Analytical data in per kg units; density not '
    a,'determined.')
 883 format(' ',7x,i1,'. Analytical data in per liter units; density '
    a,'not determined.')
 884 format(' ',7x,i1,'. Oxidized nitrogen (NO3-) recast as reduced ',
    1 'form (NH4+).')
 885 format(' ',7x,i1,'. Reduced nitrogen (NH4+) recast as oxidized ',
    1 'form (NO3-).')
 886 format(' ',7x,i1,'. Nitrate replaced by an',
    a ' equal molar quantity of bicarbonate.')
 887 format(' ',7x,i1,'. Solutes deleted: ',10a5)
 888 format(' ',7x,i1,'. Mole percent Br in Cl sites = ',
    a f6.4,'; I in Cl sites = ',f8.6,'.')
8888 format(' ',7x,i1,'. Mole percent Br in Cl sites = ',
    a f6.3,'; I in Cl sites = ',f8.5,'.')
 889 format(' ',7x,i1,'. Adjusted borate salts:',4x,a42,3x,a42)
8891 format(' ',7x,29x,a45)
 890 format(' ',7x,i1,'. Adjusted hydroxyapatite composition: ',
    a 'Ca4.75(PO4)3.17(OH).')
 892 format(' ',7x,i1,'. Salt "equiv" = total cation charge per mole ',
    a'times number of moles.')
 895 format(' ',/,33x,'NORMATIVE SALT ASSEMBLAGE INDETERMINABLE --',
    a' CALCULATION ABANDONED',/)
 901 format(' ',15x,i2,'. ',a5,4x,f9.5,4x,i3)
 902 format(' ',i2,'. ',a15,2x,a20,2x,5(2x,i2,1x,i2))
 905 format('1',56x,'SNORM DATA TABLE',/1x,/,
    a 11x,'Components',61x,'Salts',1x/,
    a 5x,7x,1x,1x,2x,'for. wt.',5x,'chg.',8x,1x,6x,
    a 4x,'name',7x,5x,1x,'chemical formula',3x,5x,3x,
    b 'component identifier with quantity',/1x)
 906 format(' ',5(1x,/))
 907 format(' ',1x,i2,'.',1x,a5,4x,f9.5,4x,i3,14x,i2,'.',1x,
    a a15,5x,a20,3x,
    b 5(3x,i2,1x,i2))
 908 format(' ',44x,i2,'.',1x,a15,5x,a20,3x,5(3x,i2,1x,i2))
 911 format(' ',/,a80)
```

```
 912 format(1x,a40,29x,a10)
 913 format(1x,79('-'))
 921 format(' ','Analysis units: ',a5,16x,'pH = ',a5,15x,
    a 'density = ',a5,/)
 925 format(' ',11x,8x,'Data',12x,'Charge adjusted',14x,'Mole ratio')
 926 format(' ',9x,2(2x,20('-')))
 927 format(' ',6x,7x,a5,6x,a5,6x,a5,6x,a5,9x,a19)
 928 format(' ',60x,a19)
 931 format(' ',1x,a5,3x,4(2x,a9),7x,a19)
 935 format(' ',9x,4(2x,9('-')),7x,a19)
 936 format(' ',3x,'Total',1x,4(2x,a9),7x,a19)
 945 format(' ',5x,'Note: borate charge of -',f5.3,' per boron.')
 947 format('No simple-salt file created.',3x)
 948 format('Simple-salt file: SS.',a10)
 950 format(' ',38x,a9,2x,3(1x,a9))
 953 format(' ','Normative salt assemblage',/,1x,25('-'))
 970 format(' ',a15,1x,a20,2x,a9,2x,3(1x,a9))
 975 format(' ',38x,9('-'),2x,3(1x,9('-')))
 976 format(' ',25x,'Total',8x,a9,2x,3(1x,a9))
 977 format(' ','Simple salts',/,1x,12('-'),/,
    a 28x,7x,6x,'percent',/,28x,7x,19('-'),/,
    b 28x,7x,3x,'mole',2x,1x,2x,'weight',/)
 978 format(' ',27x,a6,1x,a9,1x,a9)
 979 format(' ',27x,1x,'Total',1x,a9,1x,a9)
 980 format(' ','Sample ',i2,' in file: ',a10,4x,a31,5x,i2,'-',i2.2,'-'
    -,i4)
 981 format(' ',27x,6x,2(1x,9('-')))
 990 format(' ','NOTES: ',i1,'. Solute mole ratios calculated from ',
    a'initial analytical data;')
 991 format(' ',10x,'HCO3 includes CO3 via CO3 + H20 + CO2 = 2HCO3;')
 992 format(' ',10x,'alkali/halide ratio excludes lithium ',
    a'and fluoride.')
 989 format(' ',7x,i1,'. Adjusted borate salts:',4x,a42)
9891 format(' ',7x,29x,a42)
 993 format(a40,5x,a10,15x,f9.1,i1)
 994 format(8(1pe10.3))
 995 format(' ',/,7x,'NORMATIVE SALT ASSEMBLAGE INDETERMINABLE --',
    a' CALCULATION ABANDONED',/)
 996 format(a70,f9.1,i1)
     end
c*********************************************************************
```

Listing of NEODAT (File of Constants for SNORN)

```
Ca    40.08        2
Mg    24.305       2
Na    22.9898      1
K     39.0983      1
Cl    35.453      -1
SO4   96.0576     -2
PO4   94.97136    -3
CO3   60.0092     -2
Li    6.941        1
NH4   18.0383      1
NO3   62.0049     -1
Ba    137.33       2
Sr    87.62        2
B     10.811       0
F     18.9984     -1
Br    79.904      -1
I     126.9045    -1
HCO3  61.0171     -1
H2O   18.0152      0
O     15.9994      0
OH    17.00730    -1
      0.0          0
Calcite         CaCO3                01 01 08 01
Dolomite        CaMg(CO3)2           01 01 02 01 08 02
Magnesite       MgCO3                02 01 08 01
Natron          Na2CO3.10H2O         03 02 08 01 19 10
Pirssonite      Na2Ca(CO3)2.2H2O     01 01 03 02 08 02 19 02
   -            K2CO3                04 02 08 01
Strontionite    SrCO3                13 01 08 01
Witherite       BaCO3                12 01 08 01
```

```
   -           (NH4)2CO3            10 02 08 01                           0031
   -           Li2CO3               09 02 08 01                           0032
Anhydrite      CaSO4                01 01 06 01                           0033
Kieserite      MgSO4.H2O            02 01 06 01 19 01                     0034
Thenardite     Na2SO4               03 02 06 01                           0035
Arcanite       K2SO4                04 02 06 01                           0036
Glauberite     CaNa2(SO4)2          01 01 03 02 06 02                     0037
Syngenite      CaK2(SO4)2.H2O       01 01 04 02 06 02 19 01               0038
Polyhalite     Ca2K2Mg(SO4)4.2H2O   01 02 02 01 04 02 06 04 19 02         0039
Bloedite       Na2Mg(SO4)2.4H2O     02 01 03 02 06 02 19 04               0040
Leonite        K2Mg(SO4)2.4H2O      02 01 04 02 06 02 19 04               0041
Aphthitalite   K3Na(SO4)2           03 01 04 03 06 02                     0042
Celestite      SrSO4                13 01 06 01                           0043
Barite         BaSO4                12 01 06 01                           0044
Mascagnite     (NH4)2SO4            10 02 06 01                           0045
   -           Li2SO4.H2O           09 02 06 01 19 01                     0046
Antarcticite   CaCl2.6H2O           01 01 05 02 19 06                     0047
Tachyhydrite   CaMg2Cl6.12H2O       01 01 02 02 05 06 19 12               0048
Bischofite     MgCl2.6H2O           02 01 05 02 19 06                     0049
Carnallite     KMgCl3.6H2O          02 01 04 01 05 03 19 06               0050
Sylvite        KCl                  04 01 05 01                           0051
Halite         NaCl                 03 01 05 01                           0052
   -           SrCl2.2H2O           13 01 05 02 19 02                     0053
   -           BaCl2.H2O            12 01 05 02 19 01                     0054
Salammoniac    NH4Cl                10 01 05 01                           0055
   -           LiCl.H2O             09 01 05 01 19 01                     0056
Nitrocalcite   Ca(NO3)2.4H2O        01 01 11 02 19 04                     0057
Nitromagnesite Mg(NO3)2.6H2O        02 01 11 02 19 06                     0058
Niter          KNO3                 04 01 11 01                           0059
Soda Niter     NaNO3                03 01 11 01                           0060
   -           Sr(NO3)2             13 01 11 02                           0061
Nitrobarite    Ba(NO3)2             12 01 11 02                           0062
Ammonia niter  NH4NO3               10 01 11 01                           0063
   -           LiNO3.3H20           09 01 11 01 19 03                     0064
Inyoite        Ca2B6O11.13H2O       01 02 14 06 20 11 19 13               0065
Ulexite        CaNaB5O9.8H2O        01 01 03 01 14 05 20 09 19 08         0066
Indirite       Mg2B6O11.15H2O       02 02 14 06 20 11 19 15               0067
Borax          Na2B4O7.10H2O        03 02 14 04 20 07 19 10               0068
Fluorite       CaF2                 01 01 15 02                           0069
Sellaite       MgF2                 02 01 15 02                           0070
Villiaumite    NaF                  03 01 15 01                           0071
   -           LiF                  09 01 15 01                           0072
   -           Ca3(PO4)2            01 03 07 02                           0073
   -           Mg3(PO4)2            02 03 07 02                           0074
   -           Na3PO4               03 03 07 01                           0075
Fluorapatite   Ca5(PO4)3F           01 05 07 03 15 01                     0076
Wagnerite      Mg2(PO4)F            02 02 07 01 15 01                     0077
Hydroxyapatite Ca5(PO4)3OH          01 05 07 03 21 01                     0078
Inyoite**      Ca2B6O11.5H2O        01 02 14 06 20 11 19 13               0079
Ulexite**      CaNaB5O9.8H2O        01 01 03 01 14 05 20 09 19 08         0080
Indirite**     Mg2B6O11.15H2O       02 02 14 06 20 11 19 15               0081
Borax**        Na2B4O7.10H2O        03 02 14 04 20 07 19 10               0082
Kainite        KMgClSO4.11/4H2O     02 01 04 01 05 01 06 01 19 03         0083
Burkeite       Na6CO3(SO4)2         03 06 06 02 08 01                     0084
Trona          NaHCO3.Na2CO3.2H2O   03 03 08 01 18 01 19 02               0085
Kalicinite     KHCO3                04 01 18 01                           0086
TeschemacheriteNH4HCO3              10 01 18 01                           0087
   -           SrCl2.6H2O           13 01 05 02 19 06                     0088
   -           BaCl2.2H2O           12 01 05 02 19 02                     0089
Epsomite       MgSO4.7H2O           02 01 06 01 19 07                     0090
Picromerite    K2Mg(SO4)2.6H2O      02 01 04 02 06 02 19 06               0091
Gypsum         CaSO4.2H2O           01 01 06 01 19 02                     0092
Mirabilite     Na2SO4.10H2O         03 02 06 01 19 10                     0093
                                    00 00                                 0094
SIMPLE SALT    Na2Cl2               03 02 05 02                           0095
SIMPLE SALT    K2Cl2                04 02 05 02                           0096
SIMPLE SALT    MgCl2                02 01 05 02                           0097
SIMPLE SALT    CaCl2                01 01 05 02                           0098
SIMPLE SALT    CaSO4                01 01 06 01                           0099
SIMPLE SALT    MgSO4                02 01 06 01                           0100
SIMPLE SALT    K2SO4                04 02 06 01                           0101
SIMPLE SALT    Na2SO4               03 02 06 01                           0102
SIMPLE SALT    K2CO3                04 02 08 01                           0103
SIMPLE SALT    Na2CO3               03 02 08 01                           0104
SIMPLE SALT    MgCO3                02 01 08 01                           0105
SIMPLE SALT    CaCO3                01 01 08 01                           0106
                                    00 00                                 0107
**
```

APPENDIX II

Structure of SNORM

SNORM consists of a driving subroutine (MAIN), ten operational subprograms (PREP, SALWAT, LOAD, JOIN, PICK, ARRAY, CONVT, DGELG, SWAP, and PRINT), and a data bank (NEODAT) of constants for the array of solutes, salt components, and salts. The complete program listing, including NEODAT, is given in Appendix I, and the major operational features of the subprograms are summarized in table II-1.

In order to both reduce the number of solutes and salts that SNORM must distribute and identify, and expedite the calculations to identify the salts and determine their abundances, we have defined "base solutes" and "base salts." The 15 "base solutes" (table II-2) constitute an abbreviated array of the 18 SNORM solutes (table 1) that are required to define a salt assemblage; bromide and iodide are excluded as separate solutes by combining them with chloride, and bicarbonate is excluded by expressing total carbonate-bicarbonate as carbonate. Similarly, the array of 63 normative salts (table 2) is reduced to 55 "base salts" (table II-3); the reduction is accomplished by using only the lowest hydration state for each of the six pairs of normative salts with alternative hydration states (table 7), and deleting the two double-anion salts, burkeite and kainite, by considering only the Na_2CO_3-Na_2SO_4 (thenardite) and the $MgSO_4$-KCl (kieserite-sylvite) "base salt" pairs, respectively. Furthermore, each of the normative bicarbonate-bearing salts, trona, kalicinite, and teschemacherite, are expressed as their respective carbonate "base salts," and hydroxyapatite, with its modified composition (table 2), is expressed as the "base salt" $Ca_3(PO_4)_2$. With these four latter exceptions, all "base salts" are normative salts.

In identifying the proper assemblage of "base salts," the "base-salt assemblage" in JOIN (table II-1), the groups of normative salt exclusions based on gross compositional properties of the water (table 5), and the prohibited normative salt associations (table 6) are modified in SNORM (table II-4 and II-5, respectively) to reflect parallel relations among the "base salts." All equilibria defining excluded groups of "base salts" (table II-4) and prohibited "base salt" associations (table II-5) were calculated using normative salts; the "base salts" substitute for normative salts in SNORM only to expedite calculations, not to define phase equilibria. Thus, for example, the prohibited Na_2CO_3-glauberite pair is designated (table II-5) because the trona-glauberite pair reacts to form the stable calcite-thenardite or calcite-mirabilite pairs (table 6). The final set of calculations in JOIN transforms the "base-salt assemblage" into the normative salt assemblage through a series of simple exchange or hydration reactions (see SWAP in table II-1).

Table II-1. Subprograms in SNORM and their major operational features

Sub program	Major operational features
MAIN	SNORM's driver: calls PREP to enable execution, identify/create user-designated input data file, and accept user-designated options; sequentially calls LOAD and JOIN for each analysis in the file; accumulates and prints summary of number of calculations and iterations required for computing salt norm for each sample; and terminates program execution.
PREP	Called by MAIN: reads data bank (NEODAT) for solutes and salt components (table IV-2), "base" and normative salts (table IV-3), and simple salts (Appendix III); accepts identity of user-designated input data file; accepts user-designated output format(s), output character (concentration units, etc.), and, if input file already in user's directory, sample selection and solute modification options; if new data file to be entered, requests format designation (SNORM or WATEQ), calls SALWAT to create input data file with WATEQ format, requests descriptive and analytical data for water analyses and creates new input data file with SNORM format.
SALWAT	Called by PREP: requests descriptive and analytical data for water analyses and creates input data file in WATEQ format. Called by LOAD: reads one WATEQ-formatted analysis from the input data file into LOAD.
LOAD	Called by MAIN for each analysis in input data file: reads one analysis from SNORM-formatted input data file, or one WATEQ-formatted analysis from SALWAT; recasts analytical data into all possible alternative weight and mole concentrations per kilogram water, kilogram solution, and liter units; calculates carbonate fraction of analyzed bicarbonate if warrented.
JOIN	Called by MAIN: accepts data for the sample from LOAD; determines solute adjusted concentrations after incorporating user-designated solute modifications, recasting boron charge to "average" borate charge per boron, and calculating concentrations to yield charge balance between cations and anions; if compositon modifications are designated but do not affect adjusted concentration, returns to MAIN with flag to call LOAD to enter the next analysis from the input data file; recasts analysis as "base solutes" (table II-2); forms array of "eligible base salts" (see footnote 1) from listing of "base salts" (table II-3) by rejecting those "base salts" whose compositions are not represented in the analysis and those that are excluded based on gross compositional character of the water (table II-4); calculates number of "base salt" phases in a "trial base-salt assemblage;" forms all possible assemblages ("trial base salt assemblages") from the array of "eligible base salts" in which the assemblage qualitatively accomodates each base solute in the analysis and, by calling PICK, contains none of the prohibited "base

Table II-1 (continued)

Sub program	Major operational features
	salt" associations in table II-5 (see footnote 2); calculates "base salt" abundances in each successive "trial base-salt assemblage" by defining and solving a set of simultaneous equations (see footnote 3) through successively calling ARRAY, CONVT, DGELG, and CONVT; rejects "trial base-salt assemblage" that fails the test by containing one or more "base salts" with negative abundance, and returns to form and test the next "trial base-salt assemblage;" retains "trial base-salt assemblage" that yields no negative "base-salt" abundances as the "base-salt assemblage;" if the "base-salt assemblage" contains a single borate salt (or the inyoite-indirite pair), assigns correct borate charge per boron for that salt (table 3), recalculates adjusted solute concentrations to achieve charge balance, and, again calling ARRAY, CONVT, DGELG, and CONVT, recalculates salt abundances in the "base-salt assemblage" with correct stoichiometry for the borate salt; calculates a salt norm from a "base-salt" assemblage, by calling SWAP, and calculates the simple-salt assemblage from the "base-salt assemblage;" calls PRINT to format the water-sample data and results, and transmit them to the user-designated output device(s); returns to form and test remaining "trial base-salt assemblages" (see footnote 4).
PICK	Called by JOIN: tests the validity of each new "base-salt" proposal to a developing "trial base-salt assemblage" through setting a flag to reject that proposal in JOIN if the proposad salt forms any of the prohibited associations in table II-5.
ARRAY	Standard IBM software called by JOIN: recasts a two-dimensional matrix of variables (the stoichiometric abundance of each solute in each salt in a "trial base-salt assemblage") into a linear array.
CONVT	Standard IBM software called by JOIN: converts single precision variables in the linear array formed by ARRAY into double precision variables; converts the results of DGELG from double precision variables to single precision variables.
DGELG	Standart IBM software called by JOIN: solves the set of linear simultaneous equations, properly defined by ARRAY and CONVT, that equates each solute's abundance in the water to the sum of the products of the abundance of each "base salt" and that solute's stoichiometry in each salt; the results are the abundances of each of the "base salts" in the "trial base-salt assemblage."
SWAP	Called by JOIN: recasts "base-salt assemblage" into normative salt assemblage through performing the appropriate exchange reaction for each instance of (1) forming a normative double-cation salt (burkeite or kainite) from the appropriate "base salts," (2) recasting "base salt" $Ca_3(PO_4)_2$ as hydroxyapatite with modified

Table II-1 (continued)

Sub program	Major operational features
	composition, (3) recasting an alkali carbonate (table II-2) as the normative (bi)carbonate salt, (4) modifying sulfate salt associations (reactions K, J, G in table II-1) in absence of chloride and nitrate in the analysis, and (5) assigning correct hydration state to each of six pairs of alternative hydration levels (table 7).
PRINT	Called by JOIN: calculates solute molar ratios, formats and transmits water-sample data (sample descriptive data, and solute concentrations and ratios) and results of SNORM computations (identity and abundance of normative and simple salts) to the user-designated output device(s); if unable to compute norm (see footnote 4), replaces normative data with statement to that effect.

Footnotes

1. The "eligible base salts," after their designation for a given water analysis, are recast into a linear array by anion groups in the analysis (carbonates, sulfates, chlorides, nitrates, borates, and fluorides and phosphates), and assigned sequential identifier integer indices.

2. The "trial base-salt assemblages" are qualitatively formed in a sequence of nested loops; the number of loops equals the number of salts permitted in the assemblage. The value of the index in each loop is also the identifier integer of a "base salt" in the linear array of "eligible base salts;" thus, assignment of an index value to each successive loop in the heierarchy defines a full complement of base salts in the assemblage. Each loop increments through its flexible, but assigned range of indices. The limiting minimum for the indexing range in the first (outermost) loop is unity (the identifier of the first "base salt" in the linear array of "eligible base salts); in each successive (inner) loop the limiting minimum is assigned with the greater of one of two values, a value that is incremented by unity over the current index value in the preceeding (outer) loop, or, if required, a larger value that assures that each anion group in the array of eligible base salts will be represented in the full assemblage. The limiting maximum for the final (innermost) loop is the identifier integer for the last salt in the "eligible base salt" array; the limiting maximum for each of the preceeding (outer) loops is the integer that both assures enough salts remain in the array to complete the assemblage, and that each anion group will be represented in the assemblage.

   With each proposed new addition to all developing "trial base-salt assemblages," JOIN calls PICK to identify any prohibited "base-salt" associations (table II-5). If PICK flags any prohibited associations between the proposed addition and any "base salt(s)" previously assigned to the developing assemblage, the index of that loop is incremented to the

Table II-1 footnotes (continued)

next identifier integer for testing with PICK; alternatively, if the proposed new addition to the developing assemblage is not flagged by PICK (no prohibited associations), that proposed salt becomes part of the developing "trial base-salt assemblage," and each succeeding (inner) loop, following the same procedures, assigns another salt to the assemblage. After the innermost loop has been indexed and an assemblage completed, the base-salt compositions are scanned to assure each cation "base solute" in the analysis is represented in at least one "base salt;" if not, the assemblage is rejected, but if so, the assemblage is retained as a "trial base-salt assemblage." In this manner each successive "trial base-salt assemblage" is formulated with no prohibited "base-salt" associations and all "base solutes" are represented in the assemblage.

Eliminating occurrence of any prohibited associations and assuring that all solutes are represented in each "trial base-salt assemblage" markedly reduces the number of assemblages that would have been formed on a strictly mathematical basis. For example, the seawater analysis (Appendix III) with 13 "base-solute" components generates an assemblage of 12 salts with each "trial base-salt assemblage" formed from an array of 26 "eligible base salts;" mathematically, this would be represented by 9.66×10^6 different assemblages--the number of possible combinations of 26 salts taken 12 at a time. However, testing for prohibited associations 92,747 times and assuring each anion solute's representation in the assemblage produced only 1092 different assemblages; this was reduced to 567 "trial base-salt assemblages" after rejecting those assemblages that lacked one or more cation "base-solute(s)" in the resultant assemblages.

3. Salt abundances in a "trial base-salt assemblage" are determined by forming and solving a set of linear simultaneous equations. The number of equation equals the number of "base salts," N, in the assemblage. Each equation defines the quantitative distribution of a "base solute," a, throughout the "base salts" in the assemblage, and has the form

$$z_a^A m_A + z_a^B m_B + z_a^C m_C + \cdots + z_a^N m_N = M_a$$

where, in the first term on the left side of the equation, for example, z is the number of moles of "base solute" a in one formula unit of "base salt" A, m is the unknown number of moles of "base salt" A in the assemblage, and, on the right side of the equation, M is the adjusted molar concentration of "base solute" a in the analysis. Construction of (n - 1) parallel equations with n being the number of "base solutes" (chloride is normally omitted) yields a number of equations that equals the number of unknown "base-salt" abundances. The coefficients z for each term on the left side of each equation form an N x N matrix, and the (n - 1) molar abundances, M, of "base solutes" on the right side of the equations form a linear array of length N. The matrix, properly formatted in ARRAY and CONVT, is inverted in DGELG with the results of the inversion defining the "base salt" molar abundances (m_A, m_B, $m_C \cdots m_N$).

4. Two alternative outputs mark failure of SNORM to define the norm for a

Table II-1 footnotes (continued)

given water sample. First, if two or more "trial base-salt assemblages" qualify as "base-salt assemblages", each resultant "norm" is printed as though each were a different sample; such multiple norms undoubtedly signify one or more omissions from the listing of prohibited salt associations in PICK (table II-5). Second, if after testing every "trial base-salt assemblage" none qualify as a "base-salt assemblage," PRINT accepts all water-sample data from JOIN and adds the statement that the norm could not be determined. This latter result may be caused by one of two possibilities: an error in PICK (a pair of conflicting, thus unresolvable, prohibited "base salt" associations in table II-5), or, more likely, an unusual, extreme water composition whose solutes could not be quantitatively distributed into any assemblage of "base salts", such as, for example, a hypothetical K-F-rich, otherwise dilute water, but with no potassium fluoride salt in the SNORM data bank (table II-2).

Table II-2. Solutes and salt components in SNORM data file (NEODAT)

*1. Ca	*4. K	*7. PO_4	*10. NH_4	*13. Sr	16. Br	#19. H_2O
*2. Mg	*5. Cl	*8. CO_3	*11. NO_3	*14. B	17. I	#20. O
*3. Na	*6. SO_4	*9. Li	*12. Ba	*15. F	18. HCO_3	#21. OH

*"Base solutes" used in calculation of base-salt assemblage.

#Not SNORM solutes; used to calculate salt compositions and formula weights.

Table II-3. Salts in SNORM data file (NEODAT) and their chemical formulae

[Each is a normative salt unless otherwise indicated]

*1.	Calcite	$CaCO_3$	*36.	Nitromagnesite	$Mg(NO_3)_2 \cdot 6H_2O$
*2.	Dolomite	$CaMg(CO_3)_2$	*37.	Niter	KNO_3
*3.	Magnesite	$MgCO_3$	*38.	Soda niter	$NaNO_3$
*4.#	--	Na_2CO_3	*39.	--	$Sr(NO_3)_2$
*5.	Pirssonite	$Na_2Ca(CO_3)_2 \cdot 2H_2O$	*40.	Nitrobarite	$Ba(NO_3)_2$
*6.#	--	K_2CO_3	*41.	Ammonia niter	NH_4NO_3
*7.	Strontionite	$SrCO_3$	*42.	--	$LiNO_3 \cdot 3H_2O$
*8.	Witherite	$BaCO_3$	*43.	Inyoite	$Ca_2B_6O_{11} \cdot 13H_2O$
*9.#	--	$(NH_4)_2CO_3$	*44.	Ulexite	$NaCaB_5O_9 \cdot 8H_2O$
*10.	--	Li_2CO_3	*45.	Indirite	$Mg_2B_6O_{11} \cdot 15H_2O$
*11.	Anhydrite	$CaSO_4$	*46.	Borax	$Na_2B_4O_7 \cdot 10H_2O$
*12.	Kieserite	$MgSO_4 \cdot H_2O$	*47.	Fluorite	CaF_2
*13.	Thenardite	Na_2SO_4	*48.	Sellaite	MgF_2
*14.	Arcanite	K_2SO_4	*49.	Villiaumite	NaF
*15.	Glauberite	$Na_2Ca(SO_4)_2$	*50.	--	LiF
*16.	Syngenite	$K_2Ca(SO_4)_2 \cdot H_2O$	*51.#	--	$Ca_3(PO_4)_2$
*17.	Polyhalite	$K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$	*52.	--	$Mg_3(PO_4)_2$
*18.	Bloedite	$Na_2Mg(SO_4)_2 \cdot 4H_2O$	*53.	--	Na_3PO_4
*19.	Leonite	$K_2Mg(SO_4)_2 \cdot 4H_2O$	*54.	Fluorapatite	$Ca_5(PO_4)_3F$
*20.	Aphthitalite	$K_3Na(SO_4)_2$	*55.	Wagnerite	Mg_2PO_4F
*21.	Celestite	$SrSO_4$	56.@	Hydroxyapatite	$Ca_5(PO_4)_3OH$
*22.	Barite	$BaSO_4$	57.+	Inyoite	$Ca_2B_6O_{11} \cdot 13H_2O$
*23.	Mascagnite	$(NH_4)_2SO_4$	58.+	Ulexite	$NaCaB_5O_9 \cdot 8H_2O$
*24.	--	Li_2SO_4	59.+	Indirite	$Mg_2B_6O_{11} \cdot 15H_2O$
*25.	Antarcticite	$CaCl_2 \cdot 6H_2O$	60.+	Borax	$Na_2B_4O_7 \cdot 10H_2O$
*26.	Tachyhydrite	$CaMg_2Cl_6 \cdot 12H_2O$	61.	Kainite	$KMgClSO_4 \cdot 3H_2O$
*27.	Bischofite	$MgCl_2 \cdot 6H_2O$	62.	Burkeite	$Na_6CO_3(SO_4)_2$
*28.	Carnallite	$KMGCl_3 \cdot 6H_2O$	63.	Trona	$Na_3H(CO_3)_2 \cdot 2H_2O$
*29.	Sylvite	KCl	64.	Kalicinite	$KHCO_3$
*30.	Halite	$NaCl$	65.	Teschemacherite	NH_4HCO_3
*31.	--	$SrCl_2 \cdot 2H_2O$	66.	--	$SrCl_2 \cdot 6H_2O$
*32.	--	$BaCl_2 \cdot H_2O$	67.	--	$BaCl_2 \cdot 2H_2O$
*33.	Salammoniac	NH_4Cl	68.	Epsomite	$MgSO_4 \cdot 7H_2O$
*34.	--	$LiCl_2 \cdot H_2O$	69.	Picromerite	$K_2Mg(SO_2)_2 \cdot 6H_2O$
*35.	Nitrocalcite	$Ca(NO_3)_2 \cdot 4H_2O$	70.	Gypsum	$CaSO_4 \cdot 2H_2O$
			71.	Mirabilite	$Na_2SO_4 \cdot 10H_2O$

*"Base salts" used to compute the "base-salt assemblage."

#Not normative salts; included as base salt to expedite calculations.

@Hydroxyapatite calculated as $Ca_{4.75}(PO_4)_{3.17}$.

+Replace base-salt borates (43-46) if calculated with average borate charge of -7/12 (-0.583) per boron: inyoite, $Ca_{1.79}B_{6.14}O_{11}$; borax, $Na_{2.28}B_{3.91}O_7$; ulexite, $Ca_{0.98}Na_{0.98}B_{5.02}O_9$; and indirite, $Mg_{1.79}B_{6.14}O_{11}$.

Table II-4. "Base salts" excluded from trial "base salt assemblages" in SNORM as a function of charge ratios of selected cation and anion groups of solutes

[Salt numbers from table II-3]

$$[2(m_{Ca} + m_{Mg} + m_{Ba} + m_{Sr}) + m_{Li}] \,/\, [3m_{PO_4} + 2(m_{SO_4} + m_{CO_3}) + m_F + 7/12m_B{*}] > 1$$

4. Na_2CO_3
5. Pirssonite
6. K_2CO_3
8. Witherite
9. $(NH_4)_2CO_3$
13. Thenardite
14. Arcanite
15. Glauberite
16. Syngenite
18. Bloedite
19. Leonite
20. Aphthitalite
23. Mascagnite
41. Ammonia niter
44. Ulexite
46. Borax
49. Villiaumite
50. LiF
53. Na_3PO_4

$$[2(m_{Ca} + m_{Mg} + m_{Ba} + m_{Sr}) + m_{Li}] \,/\, [3m_{PO_4} + 2(m_{SO_4} + m_{CO_3}) + m_F + 7/12m_B{*}] < 1$$

25. Antarcticite
26. Tachyhydrite
27. Bischofite
31. $SrCl_2 \cdot 2H_2O$
32. $BaCl_2 \cdot H_2O$
35. Nitrocalcite
36. Nitromagnesite
39. $Sr(NO_3)_2$
40. Nitrobarite

$$[2(m_{Ca} + m_{Mg} + m_{Sr})] \,/\, [3m_{PO_4} + 2m_{CO_3}] < 1$$

11. Anhydrite
12. Kieserite
15. Glauberite
16. Syngenite
17. Polyhalite
18. Bloedite
19. Leonite
21. Celestite
28. Carnallite
43. Inyoite
44. Ulexite
45. Indirite
47. Fluorite
48. Sellaite

$$[2(m_{Ca} + m_{Mg})] \,/\, [3m_{PO_4} + 2m_{CO_3} + m_F] > 1$$

4. Na_2CO_3
5. Pirssonite
6. K_2CO_3
7. Strontionite
8. Witherite
9. $(NH_4)_2CO_3$
10. Li_2CO_3
49. Villiaumite
50. LiF
53. Na_3PO_4

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*Borate assigned an average charge of -7/12 (-0.583) per boron (see text).

APPENDIX III

User Procedures and Options

SNORM is interactive; it requests information and the user enters an appropriate response. The user creates or calls an input file containing the desired group of water analyses, and enters other parameters including the character of the output device(s), various output options, and user-elected modifications to the analyses. The results for each sample in the file are then computed and transmitted to the designated output device(s).

An example of output from SNORM is given in Appendix I for seawater. The major features of the output are: (1) title and description of the sample, and other data (density, pH, units of analysis); (2) solute data in units of the analysis and related molar and weight units, and selected molar ratios; (3) adjusted solute data in the same units as the analytical data that incorporate any user-designated solute modifications and achieve charge balance for solute distribution into the normative salts; (4) the salt norm with the concentration of each salt in the same units as listed for the solutes, and in percentage (molar and weight) of the normative assemblage with weight percentage given both in terms of the normative salts and, to more closely reflect relative solute abundances, in terms of their anhydrous stoichiometries; and (5) the simple salt assemblage as percentages (molar and weight) of each salt in the assemblage. After output for all samples in the file has been generated, a compilation of the programmatic operations that were required to calculate the norm for each sample is tabulated. For the seawater example (Appendix IV), 117,667 "salt pair tests" were made to assure no prohibited salt associations. These defined 1,954 possible potential assemblages each of which were qualitatively tested ("assemblage tests") to reject those assemblages that lacked one or more solute(s). The 851 surviving assemblages were each quantitatively tested ("inversions") to identify the single assemblage whose salt abundances could be successfully calculated (see Appendix II).

After SNORM is initiated, the program first asks the user a series of questions or requests for data to which the user replies with either appropriate integer code identifiers or, if entering new analyses, the requested descriptive and numerical data. Most user entries are displayed immediately after entry with a request for either verification of the entry or an opportunity to re-enter if an entry error was made.

Designating and creating input file

The user designates whether the norm is to be calculated from analytical data already in an existing input data file in the user's directory or from data that will be entered to create a new input file. In either case, the user then enters the name of the existing/proposed input data file. If the user designated creation of a new file but enters a file name already in the user's directory, the program requires either renaming the proposed new file or verification that that name is to be used with the result that the material currently in that file will be deleted and replaced by the new data.

If an existing data file is called, the user can elect to receive a listing of the water analyses in that file (sample number and sample description) that are sequentially numbered (locator number) in order of their occurrence in the file. The user then specifies whether the normative calculation should be made on all analyses in the file, or on only specifically designated samples in the file. If the latter option is selected, the user enters up to 25 integer values identifying the desired analyses; each integer is the locator number of an analysis in that file. With this option the normative salt calculation will be omitted for all analyses in the file that are not specifically designated; if the user mistakingly enters a locator number that exceeds the number of samples in the file, it will be ignored by SNORM. The user may also elect computation for only those analyses in the file in which the concentration of one or more (up to 10) specific solutes is given; the user designates the essential solute(s) with the result that the norm for any analysis in the file lacking data for any specified solute will not be calculated.

Creation of a new data file first requires specifying its format; the user may elect either the format that will contain only the information required by SNORM to compute the salt norm (SNORM format) or the format that will include more extensive data (redox information, concentrations of additional solutes, choice of options for calculating activity coefficients, etc.) for reading into WATEQ or WATEQF (WATEQ format). SNORM is able to create and read either format, but WATEQ and WATEQF are unable to read the SNORM format; thus, if the user anticipates a need for results from both SNORM (the salt norm) and WATEQ (mineral equilibria with the water), creating new files in the WATEQ format is recommended. The ensuing discussion, however, will be restricted to entering data in the SNORM format; the user should refer to Truesdell and Jones (1974) and Plummer and others (1976) for a discussion of WATEQ input features, procedures, and options.

SNORM's first request when creating a data input file in the SNORM format is a title for the group of analyses. This is followed by a sequence of three requests for successive one-line entries for each water analysis in the group: (1) sample number, sample pH if known, sample density if known, concentration units of solute analytical data (molality, ppm, meq/L, mg/L, or mmoles/L), and any desired short descriptive phrase about the sample or its location; (2) the concentration data for six major solutes (Ca, Mg, Na, K, Cl, and SO_4); and (3) a solute-identifier code integer and its concentration data for up to five of the remaining solutes from table 1. If data (identifier code and concentration) are entered for the last position in the entry string, the request is repeated to allow entry of the data for additional solutes; the first entry of "00" (or blank) for the solute identifier in the entry string signifies all data for that analysis have been entered and the program returns to the first of the three requests (sample number, etc.) to accept data for the next analysis. After all analyses in the group have been entered (up to 99 individual water analyses may be entered in a file), the user enters "0" (or blank) for the first of the three requests to signify completion of the new input data file. After each line of data entry when creating a new file in either the SNORM or WATEQ format, the entry is displayed and the user either acknowledges verification of the entry or requests that the line be re-entered.

Designating output devices

The user may select one or more of several possible forms for the SNORM ouptut. It may either be displayed or printed at the user's terminal at the time of executing the program, or stored as output files in the user's directory for later display or printing whenever and wherever the user specifies.

If the results are to be displayed or printed at the user's terminal at the time of program execution, one of two formats are available. The standard format uses a line-length of 131 characters that is accepted by printers with 15-inch wide paper as well as some portable printers with 8.5-inch paper and CRT display terminals. The alternative format with an 80 character line-length must be specified for many remote CRT display terminals and portable printers with 8.5-inch paper. The short line-length format is abbreviated from the standard format (Appendix IV) but no essential output is omitted; only the number of alternative concentration units for the solutes and the normative salts is reduced. The default (no user response) to this option is display/printing of the results in the standard format.

With or without immediate display/printing at the user's terminal, output can be transferred into an output data file in the user's directory for subsequent spooling to any output device with a 131 character line-length capacity (the short line-length format cannot be stored in a file). The user has the option of creating an output data file in one of two forms, or both. One form will incorporate the standard "new page" Fortran carriage control that can be implemented by some printers, particularly line printers; the second form omits the "new page" carriage control and assigns the results of each analysis to a 66 line segment (the number of lines on an 11-inch length of standard computer paper) for use on remote printers not recognizing the "new page" carriage control. Output files are named in SNORM by prefixing the input data file name with either a p. or t.; the former is assigned to an output file with carriage control, and the latter to a file without carriage control. The default for this option is to not create any output files.

A final output option, which is available if the user is entering new data to create an input data file, is to create and store the file without any output or normative calculations.

Designating character of output

The user may request a print-out of the data bank of solutes, normative salts, and simple salts (Appendix IV) to accompany the print-out of a group of salt norms. The listing of solutes consists of the chemical formula, the charge, and the gram formula weight of each. Included with the solutes are uncharged oxygen (borate formation from analyzed boron), the hydroxyl ion (hydroxyapatite formation), and molecular water (hydration water). The chemical formula, mineral name if naturally occurring, and composition in terms of moles of solute components forming its stoichiometry are listed for each normative and simple salt.

SNORM, without instructions otherwise, recasts solute and salt concentrations into the default units specified in table III-1 for output in either the standard or short line-length format. In each case, the units for salt concentrations are included in the listings of solute concentrations, and the units of both solutes and salts include the units of the original analysis. The program allows the user to override the default units and specify that salt (and solute) concentration units for all samples in the file be one of "per kilogram water," "per kilogram," or "per liter" units. Such a specification is useful, for example, if a group (file) of samples consists of analyses with with some reported in "per liter" and others reported in "per kilogram" units, and the user wishes to compare the samples or plot concentration values, common concentration units throughout the file are needed. Note, that converting from or to "per liter" units requires a density measurement; if that is lacking for any given sample, the conversion for that sample is not made and the default units are retained.

Finally, the default output of the normative assemblage includes mole concentration of each normative salt in the water sample and mole percent of each salt in the normative assemblage. The user may elect to have these values reported as salt equivalencies rather than mole units (for example, one

Table III-1. Default concentration units in SNORM output for each input concentration unit with and without density determination

Units of analysis	molality	ppm	meq/L	meq/L	mg/L	mg/L	mmol/L	mmol/L
Density determined	yes/no	yes/no	yes	no	yes	no	yes	no
Standard output format	Solutes	Solutes	Solutes	Solutes	Solutes	Solutes	Solutes	Solutes
	molal	molal	molal	meq/L	molal	meq/L	molal	meq/L
	g/kgW	g/kgW	meq/L	mmol/L	meq/L	mmol/L	meq/L	mmol/L
	mol/kg	mol/kg	mmol/L	mg/L	mmol/L	mg/L	mmol/L	mg/L
	mg/kg	mg/kg	mg/L		mg/L		mg/L	
	Salts	Salts	Salts	Salts	Salts	Salts	Salts	Salts
	molal	mol/kg	mol/L	mol/L	mol/L	mol/L	mol/L	mol/L
	mg/kgW	mg/kg	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
	mg(anhy)/kgW	mg(anhy)/kg	mg(anhy)/L	mg(anhy)/L	mg(anhy)/L	mg(anhy)/L	mg(anhy)/L	mg(anhy)/L
	mol %	mol %	mol %	mol %	mol %	mol %	mol %	mol %
	wt %	wt %	wt %	wt %	wt %	wt %	wt %	wt %
	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)
Short line-length output format	Solutes	Solutes	Solutes	Solutes	Solutes	Solutes	Solutes	Solutes
	molal	mol/kg	mmol/L	mmol/L	mmol/L	mmol/L	mmol/L	mmol/L
	g/kgW	mg/kg	meq/L	meq/L	mg/L	mg/L	mg/L	mg/L
	Salts	Salts	Salts	Salts	Salts	Salts	Salts	Salts
	molal	mol/kg	mol/L	mol/L	mol/L	mol/L	mol/L	mol/L
	mol %	mol %	mol %	mol %	mol %	mol %	mol %	mol %
	wt %	wt %	wt %	wt %	wt %	wt %	wt %	wt %
	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)	wt %(anhy)

Units: g/kgW - grams/kilogram water; meq/L - milliequivalents/liter; mg/kg - milligrams/kilogram; mg/kgW - milligrams/kilogram water; mg/L - milligrams/liter; mg(anhy)/L - milligrams anhydrous salt/liter; mg(anhy)/kg - milligrams anhydrous salt/kilogram; mg(anhy)/kgW - milligrams anhydrous salt/kilogram water; mmol/L - millimoles/liter; molal(ity) - moles/kilogram water; mol/kg - moles/kilogram; mol % - mole percent in salt assemblage; wt % - weight percent in salt assemblage; wt %(anhy) - weight percent in anhydrous salt assemblage; ppm - parts per million (mg/kg).

mole of polyhalite converts to eight equivalents, the cation charge per mole, of polyhalite). Some users may prefer this option since equivalencies among a group of salts more consistently reflect their relative abundance in the assemblage than do molar quantities.

Designating solute modifications

If salt norms are to be computed for an existing data file, the user has several options that modify the adjusted composition of the samples and the resultant normative assemblage throughout the file. These options are not available if the user is creating a new input data file because, if solute modifications are requested, norms are calculated and output generated for only those samples in the file in which the modifications have an effect.

Three of the options involve the nitrogen species, ammonia and nitrate. They form the only redox couple in SNORM and the user may wish to compare the results under alternative redox conditions. For that purpose, all nitrate can be recast as ammonia, or all ammonia as nitrate. In requesting either of these options, the user should be aware that adjusted concentrations of all solutes will be modified because recasting an anion as a cation perturbs the former charge distribution. If the user feels that nitrate in a water is a contaminant, for example, from agricultural waste, the user may elect to remove nitrate from the analysis without affecting charge distribution; this can be accomplished by requesting that nitrate be stoichiometrically replaced by bicarbonate. We selected bicarbonate because most cases of nitrate pollution occur in dilute surface waters in which bicarbonate is characteristically the dominant anion.

The fourth option eliminates any one or more (up to 10) solutes from the normative calculation by setting its concentration to 0.0 in the adjusted solute concentrations calculation. Thus, for example, nitrate (and ammonia) could be deleted from the normative calculation in this manner. As with the nitrate-ammonium exchange, use of this option will alter all adjusted solute concentrations in order to retain charge balance.

The print-out of each analysis subject to any of these solute modifications will list the water composition as originally reported in its several appropriate concentration units; only the adjusted concentrations that achieve charge balance and the resultant normative assemblage will reflect the elected modifications. Furthermore, the printout of each analysis will be footnoted as to the nature of any such modification.

APPENDIX V

Phase relations among normative salts

Each prohibited salt association in table 6 represents an equilibrium between the prohibited association and a stable, isochemical (exclusive of water and carbon dioxide) equivalent. For example, the pirssonite-magnesite pair is prohibited, and its isochemical equivalent, trona-dolomite, is stable; the equilibrium

$$\underset{\text{trona}}{2Na_3H(CO_3)_2{\cdot}2H_2O} + \underset{\text{dolomite}}{3CaMg(CO_3)_2} + H_2O \;=\; \underset{\text{pirssonite}}{3Na_2Ca(CO_3)_2{\cdot}2H_2O} + \underset{\text{magnesite}}{3MgCO_3} + CO_2$$

requires a water activity equal to or greater than 2.28 for stability of the pirssonite-magnesite pair. Such equilibria, or assumptions of equilibria if free energy data are lacking, can be used to illustrate phase relations among normative salts at 25°C, 1 bar pressure, and if carbonate-bicarbonate exchange is involved, a carbon dioxide partial pressure of $10^{-3.5}$ bars.

Some important phase relations in SNORM are shown in the following figures and tables: Ca-Mg-Na (bi)carbonates (fig. V-1); Ca-Mg-K-Na sulfates (figs. V-2 and V-3, and tables V-1 through V-4), Ca-Mg-K-Na sulfates and

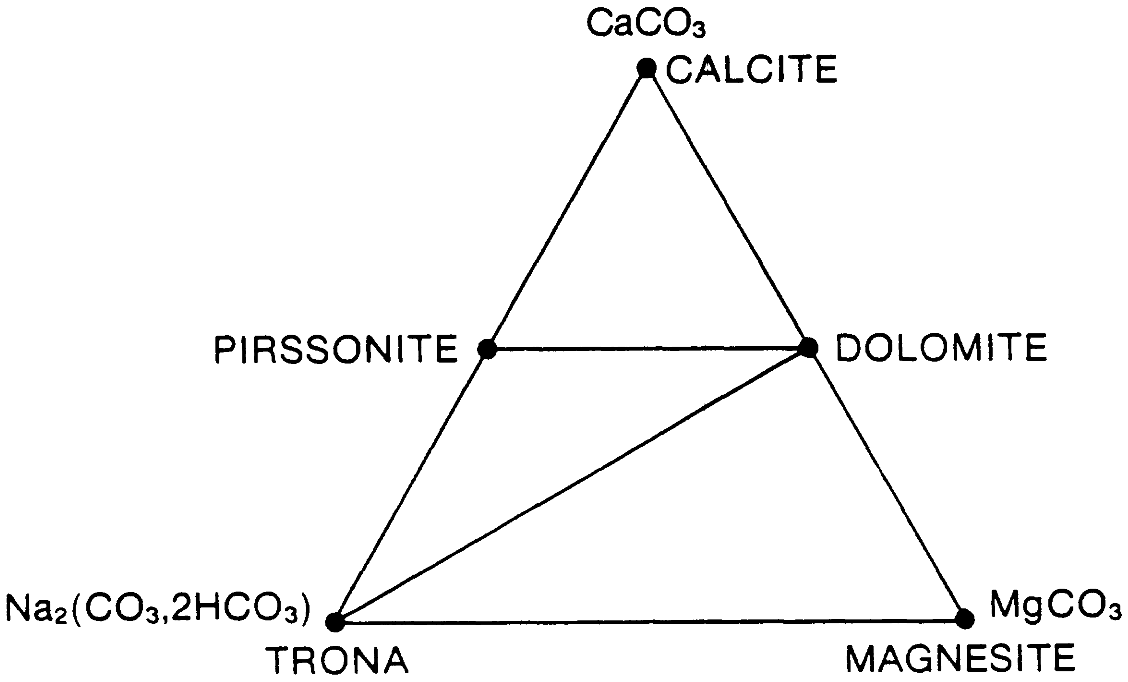

Figure V-1. Calculated phase relations among salts in the $CaCO_3$-$MgCO_3$-$Na_2(2HCO_3,CO_3)$-H_2O system at 25°C, 1 bar pressure, and $10^{-3.5}$ bars carbon dioxide partial pressure; kalicinite stable with all assemblages.

(bi)carbonates (fig. V-4), and simple-salt components of all sulfate and carbonate salts (fig. V-5); Ca-Mg-K chlorides (fig. V-6), Ca-Mg chlorides and carbonates (fig. V-7), Ca-Mg-K-Na chlorides and sulfates (fig. V-8), and simple-salt components of all chloride and carbonate salts, and all chloride and sulfate salts (fig. V-9); Ca-Mg-K nitrates and chlorides (fig. V-10), and simple-salt components of all nitrate and carbonate salts, all nitrate and sulfate salts, and all nitrate and chloride salts (fig. V-11); and Ca-Mg-Na fluorides and phosphates (fig. V-12), and Ca-Mg fluorides and carbonates, fluorides and sulfates, and fluorides and chlorides (fig. V-13). Each of these, except portions of fig. V-12, are constructed from calculated equilibria.

Figs. V-5, V-9, and V-11 identify permissible associations among the simple-salt components (with bicarbonate expressed as carbonate throughout) in normative salts for two alternative anions; the upper horizontal line is a linear array of simple-salt components of one anion and the lower horizontal line is the matching array of salts of the second anion. The diagram is to be read from left to right starting at the left end of the upper horizontal line and dropping to the lower horizontal line only after all of the anion common to the upper horizontal line has been assigned to the left-to-right sequence of salts. Thus, in fig. V-5, for example, if there is sufficient carbonate to form $MgCO_3$ and $CaCO_3$ (normative dolomite and either calcite or magnesite from fig. V-1), the simple salt component $MgSO_4$ (and any Mg-bearing normative sulfate salt from fig. V-4A) is prohibited (table 6). If unassigned carbonate remains, the next simple salt in the sequence, $SrCO_3$ (normative strontionite) forms, but if all carbonate had been assigned to Mg-Ca, $CaSO_4$ (normative anhydrite/gypsum) forms and is followed by the succeeding left-to-right sequence of sulfate simple salts until sulfate is exhausted. This type of figure is most useful in illustrating permissible (and prohibited) associations among minor cation salts or between minor cation and major cation salts.

Ca-Mg-K-Na sulfate salts

Relationships among major-cation sulfate salts are complex. A number of equilibria (table V-1) fall within the water activity interval in which salt norms occur; thus, prohibited associations (table 6) may not be valid for all norms. Harvie and others (1982) have calculated water activities in 4 sulfate-salt associations coexisting with a single chloride salt (table V-2) and 3 sulfate-salt association with two chloride salts (table V-3) in the Ca-Mg-K-Na-SO_4-Cl-H_2O system; all sulfate associations are stable within the 0.726-0.665 water activity interval between equilibria K and M (table V-1), and conform to sulfate salt phase relations in fig. V-2 and table 6. In the

Table V-1. Calculated water activities for equilibria in the $CaSO_4$-$MgSO_4$-K_2SO_4-Na_2SO_4-H_2O system at 25°C

	Reaction	a_{H_2O}*
A.	$Ca_2K_2Mg(SO_4)_4 \cdot 2H_2O + 8H_2O = MgSO_4 \cdot 7H_2O + CaSO_4 \cdot 2H_2O + K_2Ca(SO_4)_2 \cdot H_2O$ polyhalite epsomite gypsum syngenite	0.953
B.	$Na_2Ca(SO_4)_2 + 12H_2O = CaSO_4 \cdot 2H_2O + Na_2SO_4 \cdot 10H_2O$ glauberite gypsum mirabilite	0.898
C.	$Na_2Mg(SO_4)_2 \cdot 4H_2O + 13H_2O = MgSO_4 \cdot 7H_2O + Na_2SO_4 \cdot 10H_2O$ bloedite epsomite mirabilite	0.874
D.	$Na_2Mg(SO_4)_2 \cdot 4H_2O + Na_2Ca(SO_4)_2 + K_2Ca(SO_4)_2 \cdot H_2O + 17H_2O = 2NaSO_4 \cdot 10H_2O + Ca_2K_2Mg(SO_4)_4 \cdot 2H_2O$ bloedite glauberite syngenite mirabilite polyhalite	0.855
E.	$2K_3Na(SO_4)_2 + 3Na_2Mg(SO_4)_2 \cdot 4H_2O + 46H_2O = 4Na_2SO_4 \cdot 10H_2O + 3K_2Mg(SO_4)_2 \cdot 6H_2O$ aphthitalite bloedite mirabilite picromerite	0.850
F.	$K_2Mg(SO_4)_2 \cdot 6H_2O + Ca_2K_2Mg(SO_4)_4 \cdot 2H_2O + 8H_2O = 2MgSO_4 \cdot 7H_2O + 2K_2Ca(SO_4)_2 \cdot H_2O$ picromerite polyhalite epsomite syngenite	0.845
G.	$2K_3Na(SO_4)_2 + 3Na_2Ca(SO_4)_2 + 43H_2O = 4Na_2SO_4 \cdot 10H_2O + 3K_2Ca(SO_4)_2 \cdot H_2O$ aphthitalite glauberite mirabilite syngenite	0.811
J.	$2K_3Na(SO_4)_2 + 2Ca_2K_2Mg(SO_4)_4 \cdot 2H_2O + 10H_2O = Na_2Mg(SO_4)_2 \cdot 4H_2O + K_2Mg(SO_4)_2 \cdot 6H_2O + 4K_2Ca(SO_4)_2 \cdot H_2O$ aphthitalite polyhalite bloedite picromerite syngenite	0.729
K.	$CaSO_4 + Na_2Mg(SO_4)_2 \cdot 4H_2O + 3H_2O = MgSO_4 \cdot 7H_2O + Na_2Ca(SO_4)$ anhydrite bloedite epsomite glauberite	0.726
M.	$2K_3Na(SO_4)_2 + Na_2Ca(SO_4)_2 + 2Ca_2K_2Mg(SO_4)_4 \cdot 2H_2O + 9H_2O = 2Na_2Mg(SO_4)_2 \cdot 4H_2O + 5K_2Ca(SO_4)_2 \cdot H_2O$ aphthitalite glauberite polyhalite bloedite syngenite	0.665
P.	$3Ca_2K_2Mg(SO_4)_4 \cdot 2H\ O + 10Na_2SO_4 + 6H_2O = 2K_3Na(SO_4)_2 + 3Na_2Mg(SO_4)_2 \cdot 4H_2O + 6Na_2Ca(SO_4)_2$ polyhalite thenardite aphthitalite bloedite glauberite	0.463
Q.	$2K_2SO_4 + Ca_2K_2Mg(SO_4)_4 \cdot 2H_2O + 4H_2O = K_2Mg(SO_4)_2 \cdot 4H_2O + 2K_2Ca(SO_4)_2 \cdot H_2O$ arcanite polyhalite leonite syngenite	0.403
R.	$Na_2Ca(SO_4)_2 + MgSO_4 \cdot H_2O + 3H_2O = CaSO_4 + Na_2Mg(SO_4)_4 \cdot 4H_2O$ glauberite kieserite anhydrite bloedite	0.357
S.	$2K_3Na(SO_4)_2 + 4MgSO_4 \cdot H_2O + 12H_2O = Na_2Mg(SO_4)_2 \cdot 4H_2O + 3K_2Mg(SO_4)_2 \cdot 4H_2O$ aphthitalite kieserite bloedite leonite	0.305

Water activities for hydration-dehydration equilibria: H. thenardite-mirabilite at 0.805; I. anhydrite-gypsum at 0.778; L. leonite-picromerite at 0.669; N. hexahydrite-epsomite at 0.568; O. hexahydrite-kieserite at 0.498.

*Calculated equilibrium from chemical potential data in table 4.

Table V-2. Stable four-salt sulfate and coexisting chloride salt assemblages in the 25°C Ca-Mg-K-Na-SO_4-Cl-H_2O system, their equilibrium water activities from Harvie, Eugster, and Weare (1982), and the water-activity interval in which each four-salt sulfate assemblage is stable from table IV-1

	Assemblage	a_{H_2O}*	a_{H_2O}#
1.	Aphthitalite-arcanite-picromerite-syngenite-sylvite	0.777	1.000-0.403
2.	Anhydrite-glauberite-polyhalite-syngenite-halite	0.718	0.898-<0.30
3.	Aphthitalite-bloedite-glauberite-thenardite-halite	0.714	0.811-0.463
4.	Aphthitalite-bloedite-glauberite-syngenite-halite	0.711	0.811-0.665
5.	Bloedite-glauberite-polyhalite-syngenite-halite	0.708	0.855-0.665
6.	Aphthitalite-bloedite-polyhalite-syngenite-halite	0.699	0.729-0.665
7.	Aphthitalite-bloedite-picromerite-polyhalite-halite	0.684	0.729-0.665
8.	Aphthitalite-picromerite-polyhalite-syngenite-sylvite	0.675	0.729-0.403
9.	Anhydrite-bloedite-glauberite-polyhalite-halite	0.670	0.726-0.357
10.	Anhydrite-bloedite-epsomite-polyhalite-halite	0.641	0.726-0.357
11.	Bloedite-epsomite-leonite-polyhalite-halite	0.624	0.845-0.305

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*Equilibrium water activity in the 25°C Ca-Mg-K-Na-SO_2-Cl-H_2O system from Harvie, Eugster, and Weare (1982).

#Water-activity interval in which four-salt sulfate assemblage is stable from table IV-1.

Table V-3. Stable sulfate salt associations in the 25°C Ca-Mg-K-Na-SO_4-Cl-H_2O system in assemblages with two or more chloride salts, their equilibrium water activities from Harvie, Eugster, and Weare (1982), and the water-activity intervals in which the sulfate salt associations are stable from table IV-1

	Sulfate assemblage	$a_{H_2O}^{*}$	$a_{H_2O}^{\#}$
1.	Anhydrite-polyhalite-syngenite-halite-sylvite	0.682	0.953-<0.30
2.	Aphthitalite-polyhalite-syngenite-halite-sylvite	0.674	0.729-<0.30
3.	Aphthitalite-picromerite-polyhalite-halite-sylvite	0.672	0.729-<0.30
4.	Epsomite-leonite-polyhalite-kainite-halite	0.605	0.845-<0.30
5.	Leonite-polyhalite-kainite-halite-sylvite	0.605	0.845-<0.30
6.	Anhydrite-polyhalite-carnallite-halite-sylvite	0.521	0.953-<0.30
7.	Polyhalite-kainite-carnallite-halite-sylvite	0.518	0.953-<0.30
8.	Kieserite-polyhalite-kainite-carnallite-halite	0.469	0.953-<0.30
9.	Anhydrite-kieserite-polyhalite-carnallite-halite	0.459	0.953-<0.30
10.	Anhydrite-kieserite-bischofite-carnallite-halite	0.338	>0.95-<0.30

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[*] Equilibrium water activity in the 25°C Ca-Mg-K-Na-SO_4-Cl-H_2O system from Harvie, Eugster, and Weare (1982).

[#] Water activity interval in which the sulfate salt association (excluding single-salt hydration-dehydration equilibria) is stable from table IV-1.

Table V-4. Stable four-salt sulfate assemblages in the 25°C $CaSO_4$-$MgSO_4$-K_2SO_4-Na_2SO_4-H_2O system, their equilibrium water activities from Harvie, Eugster, and Weare (1982), and the water-activity interval in which each four-salt sulfate assemblage is stable from table IV-1

	Sulfate assemblage	a_{H_2O}[*]	a_{H_2O}[#]
1.[+]	Aphthitalite-arcanite-picromerite-syngenite	0.934	1.000-0.403
2.[+]	Glauberite-gypsum-polyhalite-syngenite	0.870	0.898-<0.30
3.	Epsomite-glauberite-gypsum-polyhalite	0.840	0.898-0.726
4.[+]	Bloedite-glauberite-polyhalite-syngenite	0.832	0.855-0.665
5.	Bloedite-epsomite-glauberite-polyhalite	0.831	0.874-0.726
6.	Bloedite-glauberite-mirabilite-syngenite	0.830	0.855-0.811
7.	Aphthitalite-bloedite-mirabilite-syngenite	0.827	0.850-0.811
8.	Aphthitalite-bloedite-picromerite-syngenite	0.826	0.850-0.729
9.	Bloedite-picromerite-polyhalite-syngenite	0.824	0.845-0.729
10.[+]	Bloedite-epsomite-picromerite-polyhalite	0.822	0.845-0.305

[*] Equilibrium water activity in the 25°C $CaSO_4$-$MgSO_4$-K_2SO_4-Na_2SO_4-H_2O system from Harvie, Eugster, and Weare (1982).

[#] Water-activity interval in which four-salt sulfate assemblage is stable from table IV-1.

[+] Stable assemblages in chloride-bearing system (table 9) except for appropriate single-salt hydration reactions.

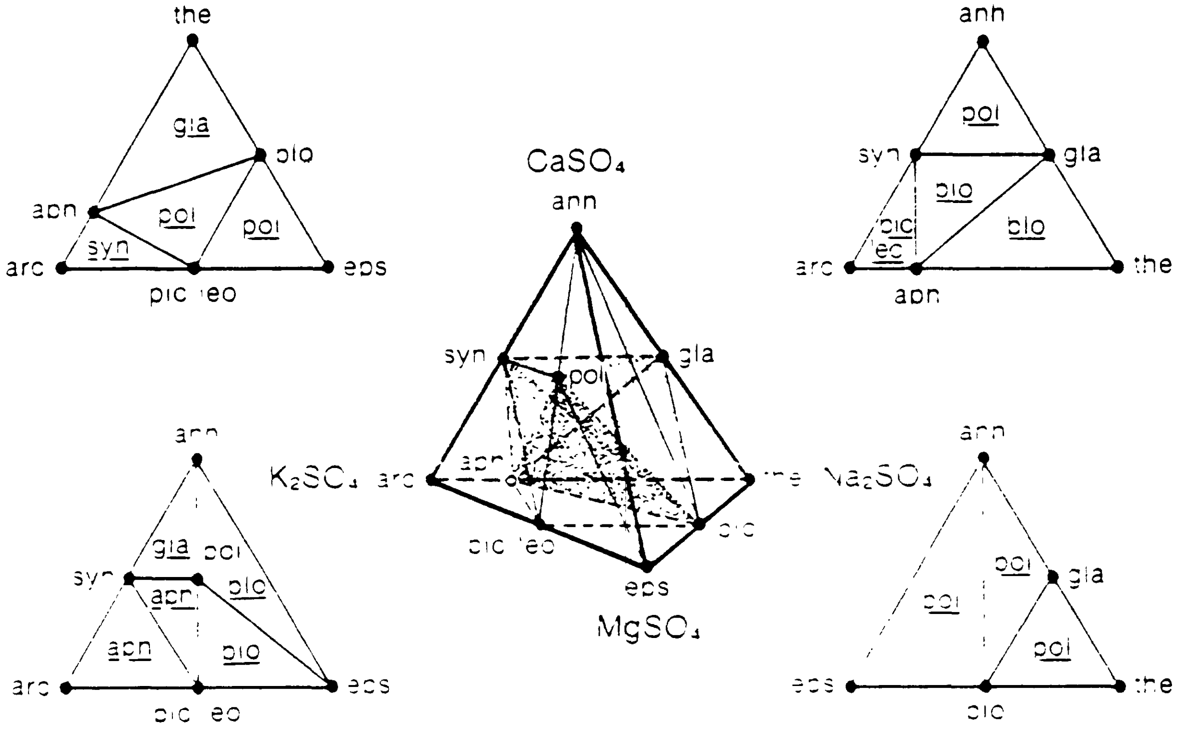

Figure V-2. Calculated phase relations in the $CaSO_4$-$MgSO_4$-K_2SO_4-Na_2SO_4-H_2O system at 25°C and 1 bar pressure within the water activity interval between 0.726 and 0.665 that represents normative salt relations in chloride or nitrate bearing waters; interval includes the picromerite-leonite transition (a_{H_2O}=0.669). Central tetrahedron is projection of the five-component system into the quaternary sulfate salt tetrahedron; the four surrounding sulfate salt ternaries are faces of the tetrahedron. Mineral abbreviations from table 2; underlined abbreviation within each three-phase association on the ternary faces identify stable salt containing the fourth sulfate component. Solid joins on exposed faces of tetrahedron, dashed joins on hidden faces, and dotted joins penetrate tetrahedron; highlighted assemblages (aph-blo-pol-syn and blo-gla-pol-syn) do not form a three-phase association on any ternary face.

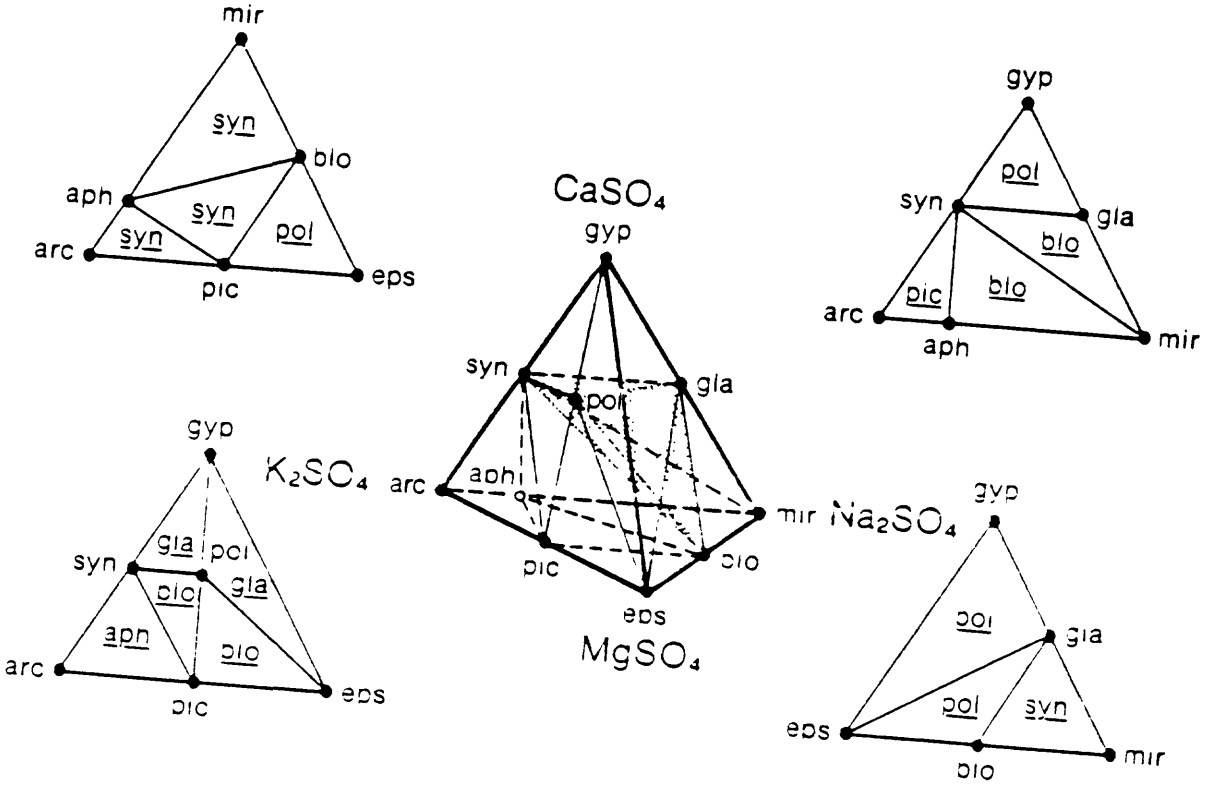

Figure V-3. Calculated phase relations in the $CaSO_4$-$MgSO_4$-K_2SO_4-Na_2SO_4-H_2O system at 25°C and 1 bar pressure within the water activity interval between 0.845 and 0.811 that represents normative salt relations in waters lacking chloride and nitrate. Central tetrahedron is projection of the five-component system into the quaternary sulfate salt tetrahedron; the four surrounding sulfate salt ternaries are faces of the tetrahedron. Mineral abbreviations from table 2; underlined abbreviation within each three-phase association on the ternary faces identify stable salt containing the fourth sulfate component. Solid joins on exposed faces of tetrahedron, dashed joins on hidden faces, and dotted joins penetrate tetrahedron; highlighted assemblage (blo-gla-pol-syn) does not form a three-phase association on any ternary face.

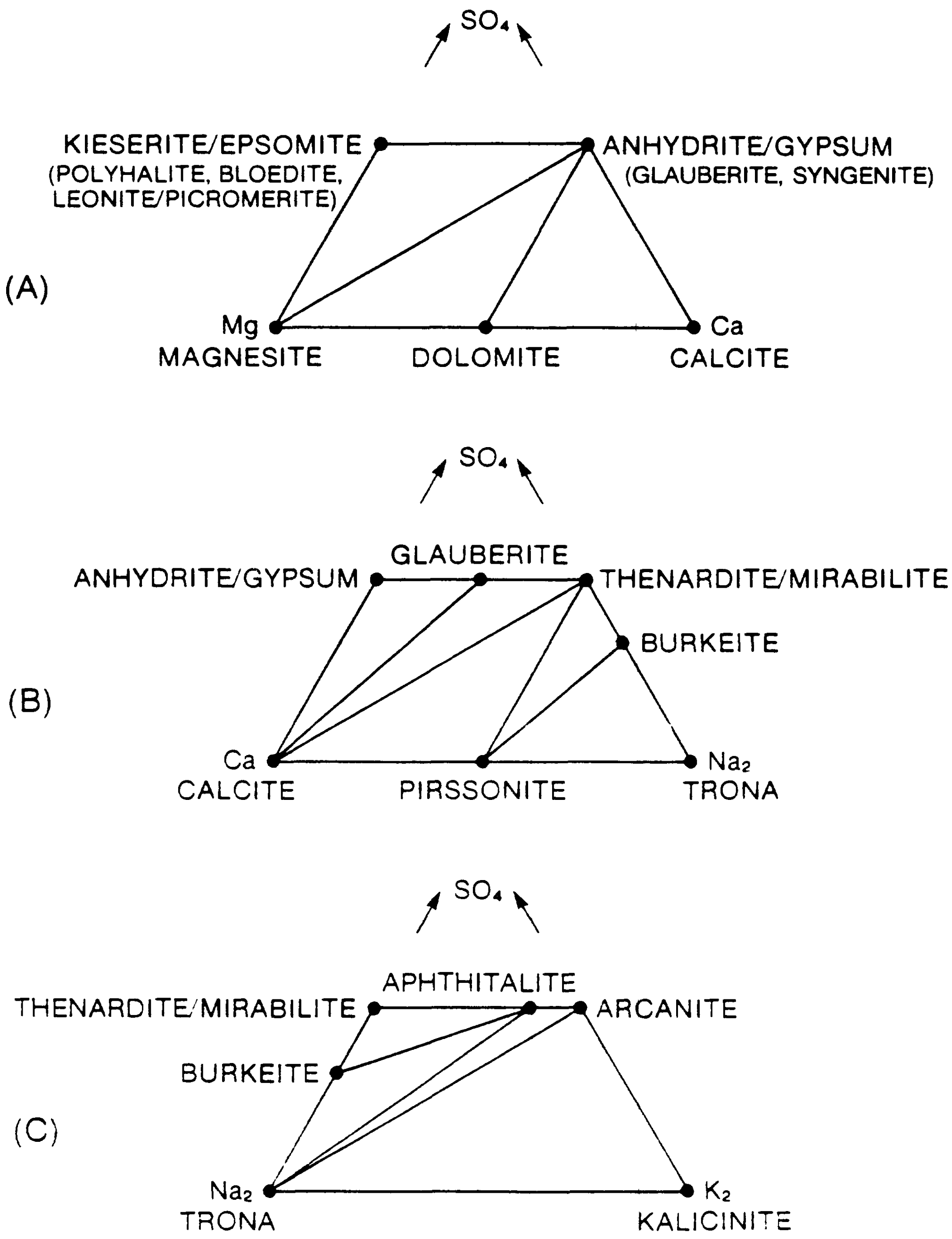

Figure V-4. Calculated phase relations among (bi)carbonate and sulfate normative salts at 25°C, 1 bar pressure, and $10^{-3.5}$ bars partial pressure of CO_2 in (bi)carbonate-saturated assemblages with sulfate and two cations: (A) $Mg-Ca-SO_4-CO_3-H_2O$ system with permissable alkali-bearing sulfates in parentheses; (B) $Ca-Na_2-SO_4-(CO_3,2HCO_3)-H_2O$ system; and (C) $Na_2-K_2-SO_4-(CO_3,2HCO_3)-H_2O$ system.

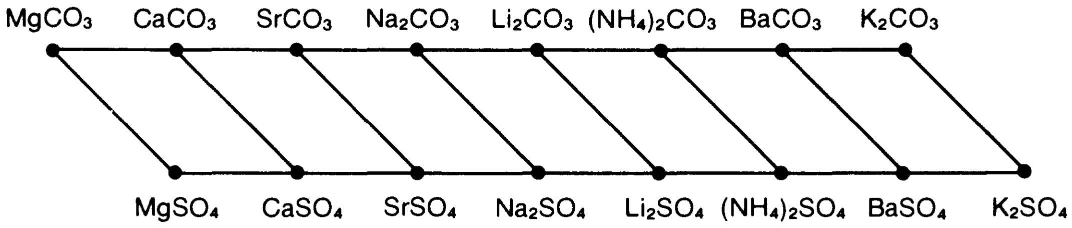

Figure V-5. Calculated relations at 25°C, 1 bar pressure, and $10^{-3.5}$ bars CO_2 partial pressure among carbonate and sulfate simple-salt components of normative salts with permissable associations forming a path that proceeds only from left to right on the diagram; bicarbonate components included with carbonate components.

absence of chloride and nitrate (unknown to our knowledge in natural waters), the stable 4 sulfate-salt assemblages and their water activities (Harvie and others, 1982) are stable in the 0.845-0.811 water activity interval (table V-4) between equilibria F and G (table V-1) and conform to phase relations in Fig. V-3. A hypothetical chloride-nitrate free water prompts SNORM to perform reactions K, J, and G (table V-1) to form major-cation sulfate associations that are in accordance with table 6 and fig. V-2, to yield the correct associations.

Ca-Mg-Na borate salts

Because free energy values for three of the four normative borate salts are lacking, the prohibited associations of borate salts in the salt norm are assigned to conform with general relations observed in natural assemblages and be consistent with relations in other salt groups.

We have restricted indirite's occurrence to Mg-rich norms in which magnesite is the sole carbonate; anhydrite, kieserite, leonite/picromerite, and polyhalite are the only permissible sulfates; bischofite and carnallite are the only permissible Ca and Mg-bearing chlorides; and nitromagnesite is the only permitted Ca and Mg-bearing nitrate. These relations were assigned based on the dominance, albeit secondary origin, of the magnesium borates boracite and ascherite in marine evaporites, the occurrence of indirite and kurnakovite in the Indir salt dome in Russia (Kühn, 1968; Braitsch, 1971; Sonnenfeld, 1984), and the paucity and nearly exclusively secondary origin of indirite and other magnesium borates in continental playa deposits (Muessig, 1959, 1966; Bowser and Dickson, 1966).

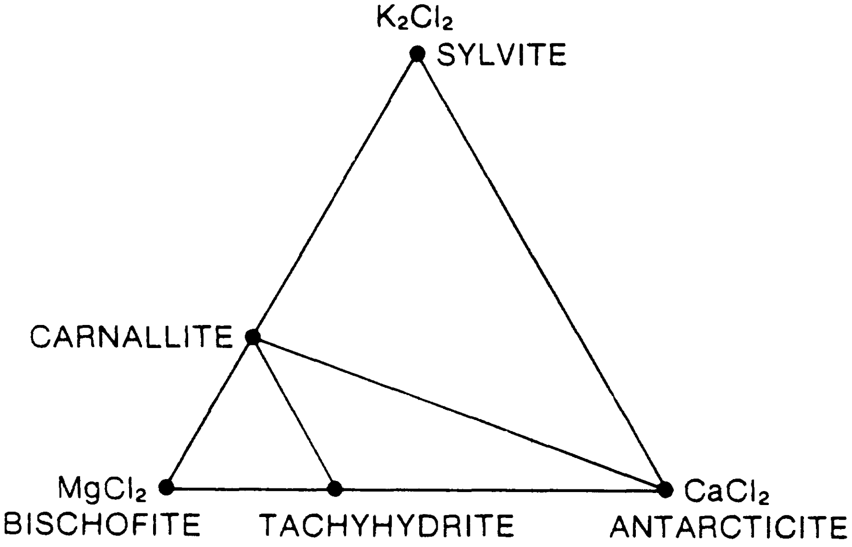

Figure V-6. Calculated phase relations among normative salts in the $CaCl_2$-$MgCl_2$-K_2Cl_2-H_2O system at 25°C and 1 bar pressure; coexisting halite stable with all assemblages.

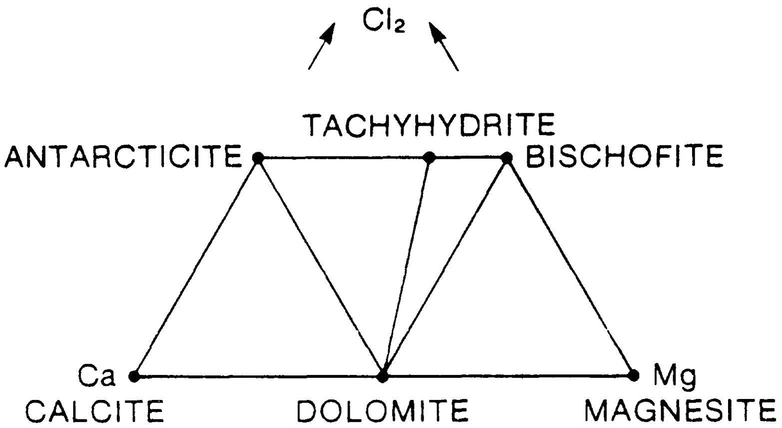

Figure V-7. Calculated phase relations among normative salts in the Ca-Mg-Cl_2-CO_3-H_2O system at 25°C, 1 bar pressure, and $10^{-3.5}$ bars CO_2 partial pressure with carnallite and halite permissable coexisting K and Na salts.

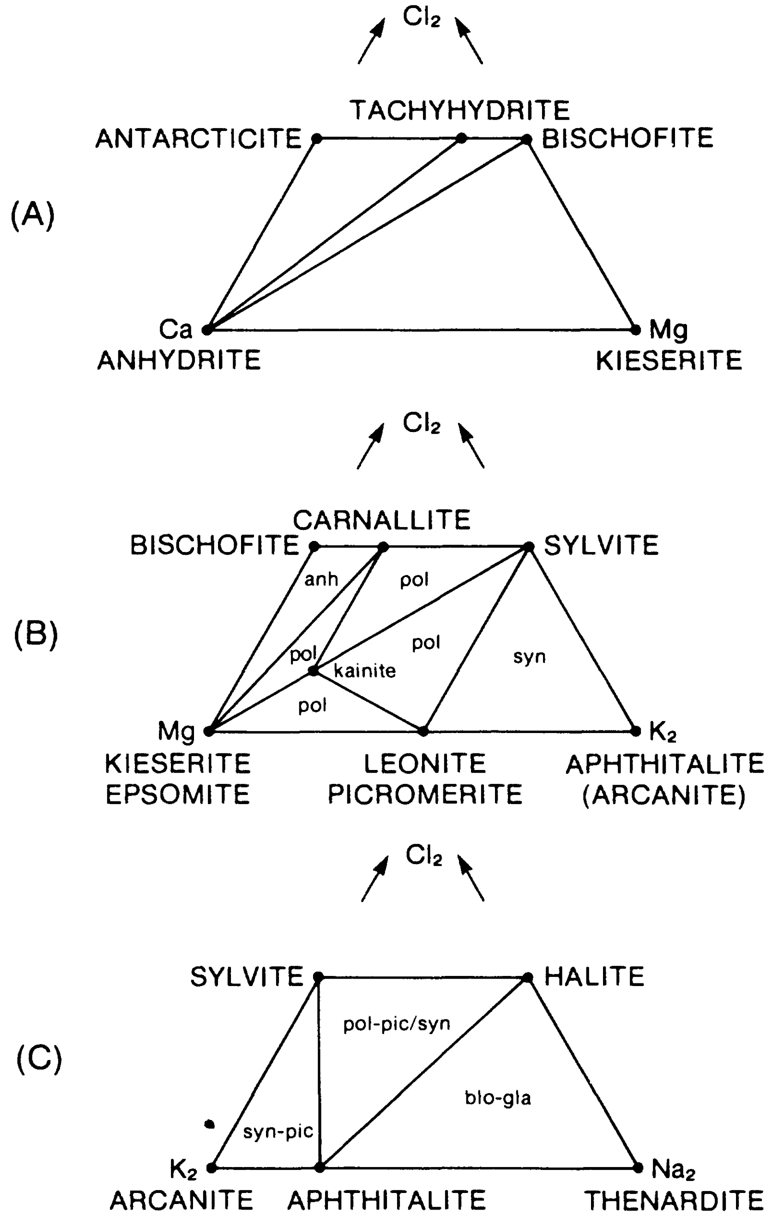

Figure V-8. Calculated phase relations among sulfate and chloride normative salts at 25°C and 1 bar pressure in sulfate-saturated assemblages with chloride and two cations; salt abbreviations from table 2: (A) Ca-Mg-Cl_2-SO_4-H_2O system with carnallite and halite as permissable coexisting K and Na salts; (B) Mg-K_2-Cl_2-SO_4-H_2O system with sulfates labeled in three-phase triangles and halite permissable coexisting Ca and Na salts (if arcanite-aphthitalite present halite not permitted, see (C) below); and (C) K_2-N_2-Cl_2-SO_4-H_2O system with sulfates labeled in three-phase triangles permissable coexisting Ca and Mg salts.

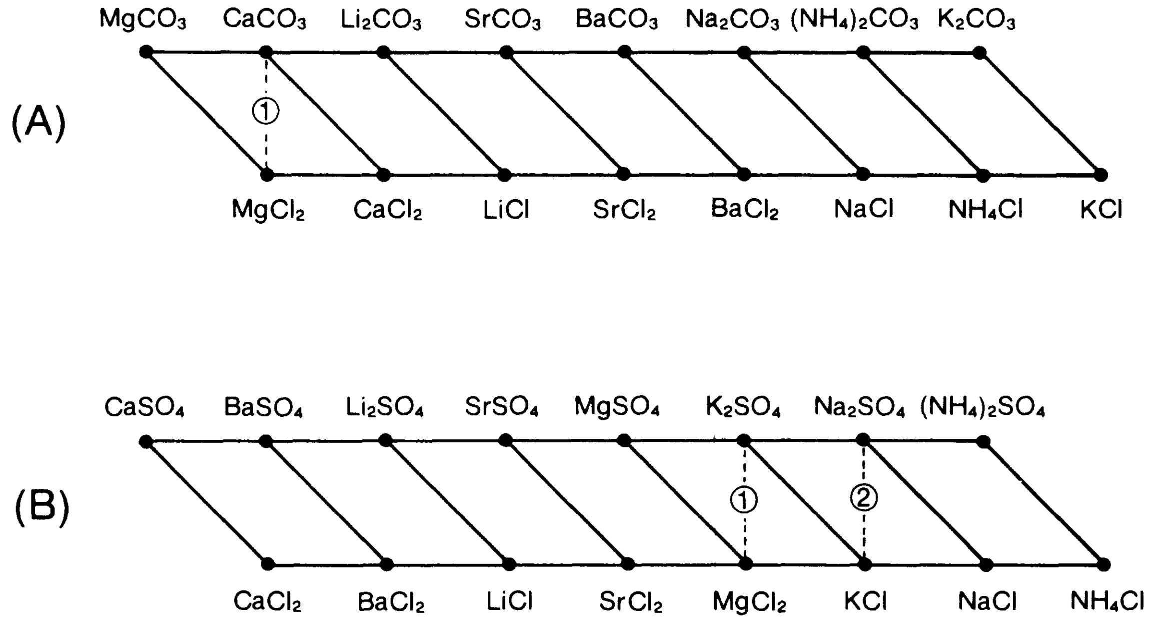

Figure V-9. Calculated relations among simple-salt components of normative salts with permissable associations at 25°C, 1 bar pressure, and $10^{-3.5}$ bars CO_2 partial pressure forming a path that proceeds only from left to right on each diagram: (A) (bi)carbonate and chloride salt components with bicarbonate components included with carbonate components and dashed segment 1 denoting stability of the dolomite-tachyhydrite pair; (B) sulfate and chloride salt components with dashed segment 1 denoting stability of the carnallite-polyhalite pair and dashed segment 2 denoting stability of the aphthitalite-sylvite pair.

Normative inyoite is also similarly restricted but to Ca-rich norms; one or more of Ca-bearing chlorides and nitrates, and Sr and Ba chlorides and nitrates characteristically coexist with inyouite, and anhydrite is the only major-cation sulfate that is permitted in inyoite-bearing assemblages. Primary calcium borate minerals are rare in continental evaporite deposits although colemanite and, to a lesser extent, inyoite and meyerhofferite are observed as secondary minerals in some lacustrine assemblages (Muessig, 1959; Bowser and Dickson, 1966); documented primary inyoite has only been described from a single continental deposit--Laguna Salinas, Peru (Muessig, 1958).

By far the dominant minerals in continental playa and thermal spring deposits are borax and ulexite; they are the normative borates that occur in norms of typical continental waters generally characterized by normative alkali-bearing sulfates and possibly (bi)carbonates. We have arbitrarily established the following criteria for their occurrence in normative

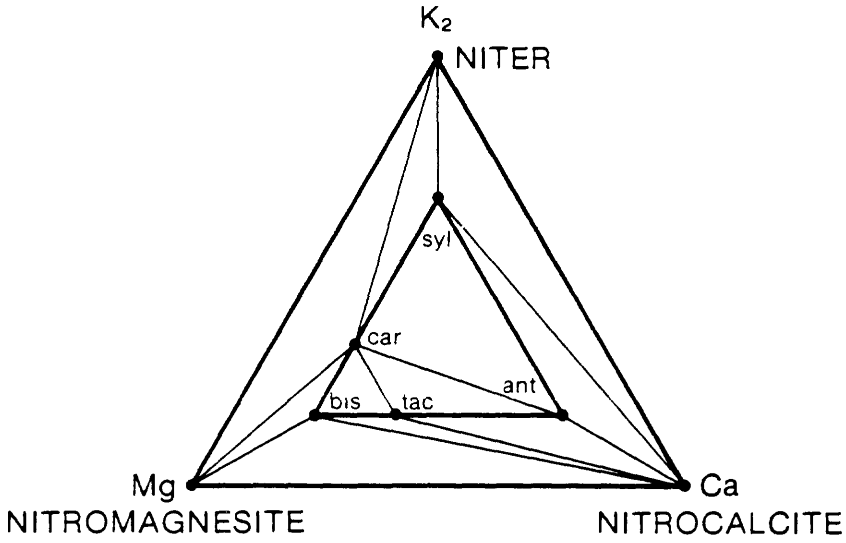

Figure V-10. Calculated phase relations among normative salts in the Ca-Mg-K-Cl-NO_3-H_2O system at 25°C and 1 bar pressure in nitrate-saturated assemblages looking down onto the Cl_2-K_2-Ca-Mg tetrahedron with the Cl_2 apex truncated along the K_2Cl_2-$CaCl_2$-$MgCl_2$ plane; salt abbreviations from table 2; halite occurs with all assemblages as the permissable sodium salt except for the prohibited niter-nitromagnesite-halite association that is replaced by the soda niter-carnallite pair.

assemblages: neither borax nor ulexite are permitted to coexist with any Ca and Mg-bearing chloride and nitrate salts (inyoite and indirite occur in such assemblages); only borax coexists with any Na-bearing (bi)carbonate salt (pirssonite, trona, burkeite) or Na-bearing alkali sulfate salt (thenardite/mirabilite, aphthitalite); and only ulexite occurs with anhydrite, kieserite/epsomite, and the polyhalite-glauberite pair unless either inyoite or indirite is the proper borate salt (table 6).

These criteria for the occurrence of borax and ulexite appear, in general, to be compatable with borate mineral occurrences in Quaternary playa and thermal spring deposits. Other than searlesite (a sodium borosilicate), the only borate minerals in the Searles Lake evaporites are borax and its less hydrated analog, tincalconite associated with one or more of gaylussite, pirssonite, trona, nahcolite, thenardite, and mirabilite; Ca-bearing borates are not observed (Smith and Haines, 1964). In the numerous and extensive playa and thermal spring deposits in the high Andes of South America (Muessig, 1958, 1959, 1966; Rettig and others, 1980), on the other hand, ulexite is the dominant primary borate, borax is infrequently abundant, and primary inyoite

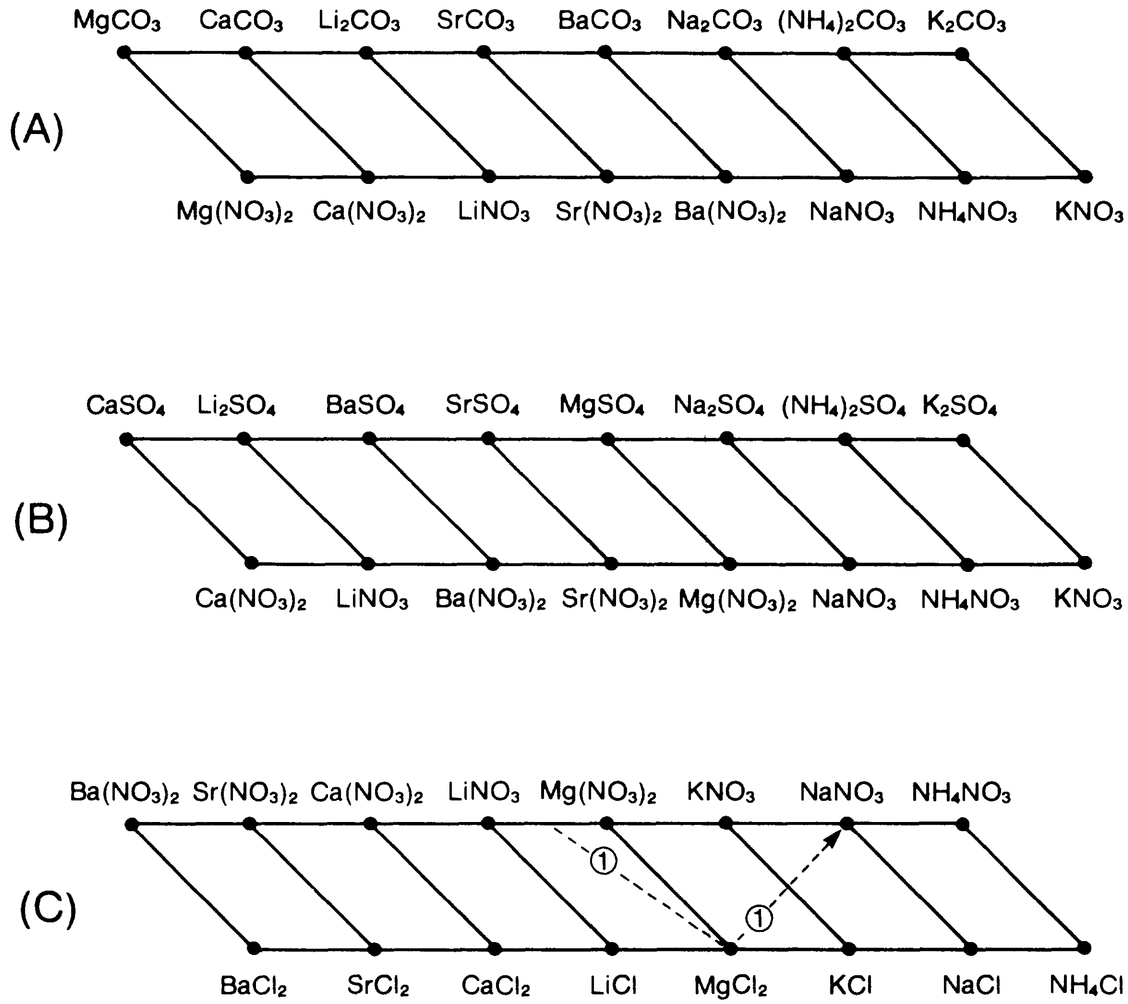

Figure V-11. Calculated relations among simple-salt components of normative salts at $25^{\circ}C$, 1 bar pressure, and $10^{-3.5}$ bars CO_2 partial pressure with permissable associations forming a path that proceeds only from left to right on the diagram: (A) (bi)carbonate and nitrate salt components with bicabonate components included with carbonate components; (B) sulfate-nitrate salt components; and (C) nitrate-chloride salt components with dashed segment 1 denoting stability of the soda niter-carnallite pair.

and indirite are rarely observed; a very common association in many of these deposits is the ulexite-gypsum pair.

We recognize that the mineral associations assigned to SNORM are far more rigorous and specific than those observed in natural associations; however, in order for SNORM to define a single normative assemblage for a boron-bearing water, comprehensive restrictions (table 6) must be imposed. We feel our assignments are not in conflict with relations in naturally occurring assemblages, but, at the same time, they are subject to modifications as more definitve observations become available or themodynamic data for additional borate mineral salts are determined.

Ca-Mg-Na phosphate and fluoride salts

Fig. V-12 is constructed with Na_3PO_4 and $Mg_3(PO_4)_2$ as nonmineral salts. We exclude the former from all assemblages that contain suffcient Ca and Mg to form their respective phosphates, and permit the latter only if insufficient fluoride exists to form wagnerite. Because the free energy of wagnerite is unknown, we have assumed stability of the fluorapatite-sellaite pair and prohibited the wagnerite-fluorite pair; sellaite is more widespread than wagnerite in marine evaporites and apparently coexists with fluorapatite (Kühn, 1968; Braitsch, 1971, Sonnenfeld, 1984). Fortunately standard free engergies of the Ca-Mg-Na fluorides are available (table 4) that allow determination of their equilibria (fig. V-13), and the restriction of LiF and villiaumite to alkali-bearing (bi)carbonate associations with LiF-trona being stable with respect to villiaumite-Li_2CO_3. Phosphate and fluorphosphate normative mineral assignments are assumed to have restrictions that parallel

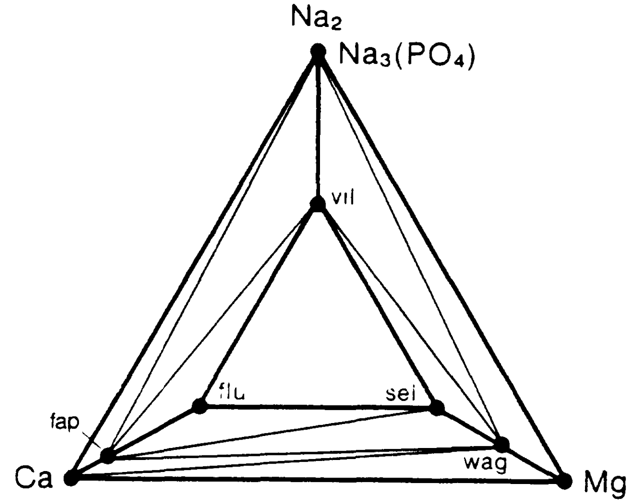

Figure V-12. Suggested phase relations among normative salts in the Ca-Mg-Na-PO_4-F-H_2O system at 25°C and 1 bar pressure projected into the phosphate and water saturated F_2-Na_2-Ca-Mg tetrahedron with the F_2 apex truncated along the Na_2F_2-CaF_2-MgF_2 plane. Salt mineral abbreviations from table 2; hydroxyapatite plotted as $Ca_3(PO_4)_2$.

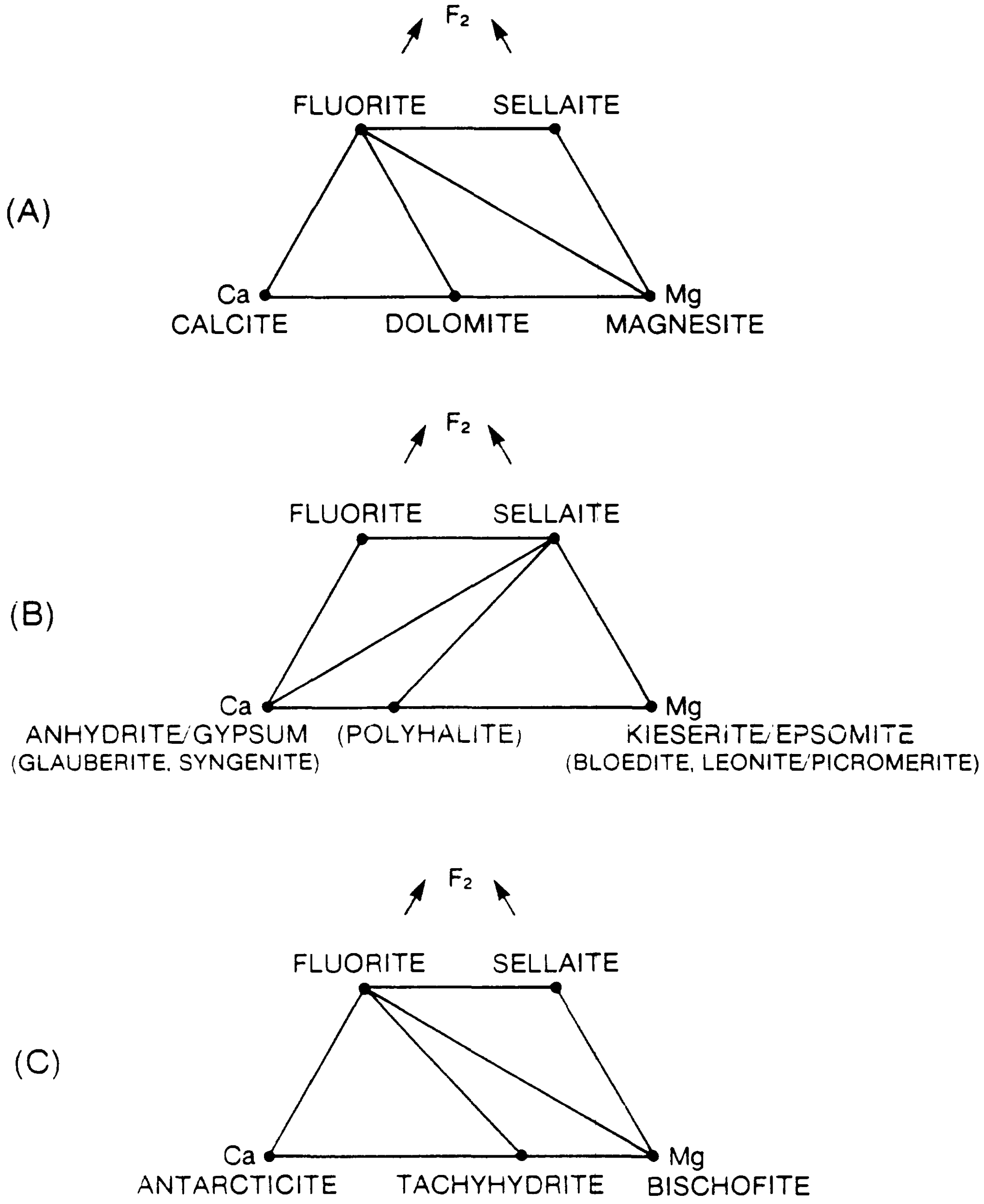

Figure V-13. Calculated phase relations among Ca-Mg fluoride salts and coexisting carbonate, sulfate, and chloride salts at 25°C and 1 bar pressure projected onto the Ca-Mg-F_2 triangle and saturated with the major anion and water: (A) Ca-Mg-CO_3-F_2-H_2O system at CO_2 partial pressure of $10^{-3.5}$ bars; (B) Ca-Mg-SO_4-F_2-H_2O system; and (C) Ca-Mg-Cl_2-F_2-H_2O system. Mineral compositions in parentheses lie outside of the designated system; Ca-Mg phosphates and fluorphosphates suggested to have identical relations with major anion salts as the fluorides.

Table V-5. Prohibited salt associations (table 6) involving three or more anions and their permissable isochemical equivalents

	Prohibited association	Permissable isochemical equivalent
A.	bischofite-celestite-dolomite	$SrCl_2 \cdot nH_2O$-anhydrite-magnesite
B.	carnallite-celestite-calcite	$SrCl_2 \cdot nH_2O$-sylvite-anhydrite-dolomite
C.	$BaCl_2 \cdot nH_2O$-anhydrite-magnesite	bischofite-barite-dolomite
D.	nitrocalcite-sylvite-magnesite	niter-carnallite-dolomite
E.	niter-carnallite-calcite	nitrocalcite-sylvite-dolomite
F.	soda niter-carnallite-dolomite	niter-nitrocalcite-halite-magnesite
G.	soda niter-carnallite-calcite	nitrocalcite-sylvite-halite-dolomite
H.	ulexite-$SrCl_2 \cdot nH_2O$-anhydrite	inyoite-halite-celestite
I.	inyoite-syngenite-halite	ulexite-anhydrite-sylvite
J.	indirite-$SrCl_2 \cdot nH_2O$-anhydrite	inyoite-bischofite-celestite
K.	indirite-syngenite-halite	ulexite-polyhalite-sylvite
L.	sellaite-$SrCl_2 \cdot nH_2O$-anhydrite	fluorite-bischofite-celestite
M.	$Mg_3(PO_4)_2$-$SrCl_2 \cdot nH_2O$-anhydrite	hydroxyapatite-bischofite-celestite
N.	wagnerite-$SrCl_2 \cdot nH_2O$-anhydrite	fluorapatite-fluorite-bischofite-celestite
O.	$SrCl_2 \cdot nH_2O$-sylvite-anhydrite-magnesite	carnallite-celestite-dolomite
P.	$BaCl_2 \cdot nH_2O$-sylvite-anhydrite-dolomite	carnallite-barite-magnesite
Q.	$Sr(NO_3)_2$-carnallite-barite-calcite	nitrobarite-$SrCl_2 \cdot nH_2O$-sylvite-anhydrite-dolomite
R.	nitrobarite-sylvite-anhydrite-magnesite	niter-carnallite-barite-dolomite

H, I, J, K -- Ba can substitute for Sr in $SrCl_2 \cdot nH_2O$ and yield barite rather than celestite; NO_3 can substitute for Cl in $(Sr/Ba)Cl_2 \cdot nH_2O$ and yield soda niter (N) or nitromagnesite (O, P, Q, R) rather than or bischofite.

the fluorides, except, whenever possible, prohibiting Na_3PO_4 in favor of the apatite-trona and wagnerite-trona pairs.

Equilibria involving three anions

Many of the three and four salt association in table 6 contain three or more anions; each is listed in table V-5 along with it isochemically equivalent permissible association. Each involves a minor solute and, to a large extent, each is an extension of a related two-anion association.

For example, the tachyhydrite-celestite association is prohibited (table 6) in favor of the stable bischofite-anhydrite-$SrCl_2 \cdot 2H_2O$ association (fig. V-9). If there is insufficient tachyhydrite to convert all celestite to $SrCl_2 \cdot 2H_2O$, the bishofite and celestite can interact with dolomite (the stable carbonate with tachyhydrite) to convert more celestite to $SrCL_2 \cdot 2H_2O$ and yield anyhdrite and magnesite (A in table V-5). However, the parallel sequence of associations with barium salts rather than strontium, although again prohibiting the barite-tachyhydrite association (table 6 and fig. V-9), permits the bischofite-barite-dolomite association and prohibits the $BaCl_2 \cdot 2H_2O$-anhydrite-magnesite association (C in table V-5).

APPENDIX IV

Examples of SNORM Output--Short Line-Length Format

```
COMPOSITION OF SEAWATER
Riley & Chester (1971); Wedepohl (1971)                              Sea water
-------------------------------------------------------------------------------
Analysis units: mg/kg                pH =  8.00               density = 1.030

                   Data            Charge adjusted             Mole ratio
           --------------------  --------------------
              M/kg      mg/kg       M/kg      mg/kg              Ca/Mg 1.93E-01
                                                                  K/Na 2.18E-02
 Mg        5.320E-02  1.293E+03  5.322E-02  1.293E+03       Mg+Ca/Na+K 1.33E-01
 Ca        1.025E-02  4.110E+02  1.026E-02  4.111E+02        alk./hal. 8.75E-01
 Sr        9.016E-05  7.900E+00  9.019E-05  7.902E+00          HCO3/Cl 4.29E-03
 Ba        9.466E-08  1.300E-02  9.469E-08  1.300E-02           SO4/Cl 5.17E-02
 Li        2.881E-05  2.000E-01  2.882E-05  2.001E-01             F/Cl 1.23E-04
 Na        4.681E-01  1.076E+04  4.683E-01  1.077E+04            Br/Cl 1.54E-03
 K         1.021E-02  3.990E+02  1.021E-02  3.991E+02             I/Cl 7.22E-07
 F         6.737E-05  1.280E+00  6.735E-05  1.280E+00           PO4/Cl 3.86E-06
 Cl        5.459E-01  1.935E+04  5.457E-01  1.938E+04             B/Cl 7.54E-04
 Br        8.423E-04  6.730E+01  8.419E-04  6.727E+01            Mg/Cl 9.75E-02
 I         3.940E-07  5.000E-02  3.939E-07  4.998E-02            Ca/Cl 1.88E-02
 HCO3      2.344E-03  1.430E+02  2.307E-03  1.408E+02            Sr/Cl 1.65E-04
 CO3           -          -      3.576E-05  2.146E+00            Ba/Cl 1.73E-07
 SO4       2.820E-02  2.709E+03  2.819E-02  2.708E+03            Li/Cl 5.28E-05
 B         4.116E-04  4.450E+00  4.115E-04  4.448E+00            Na/Cl 8.58E-01
 PO4       2.106E-06  2.000E-01  2.105E-06  1.999E-01             K/Cl 1.87E-02
           ---------  ---------  ---------  ---------
   Total   1.120E+00  3.515E+04  1.120E+00  3.518E+04
     Charge balance:  sum[+]/sum[-] = 0.9993
     Note: borate charge of -0.667 per boron.

Normative salt assemblage
-------------------------
                                        mol/kg      %(mol)     %(wt)   %(an-wt)

Halite          NaCl                  4.683E-01    88.05749  70.06436  78.08681
Bischofite      MgCl2.6H2O            2.381E-02     4.47838  12.38930   6.47149
Carnallite      KMgCl3.6H2O           1.021E-02     1.91966   7.25858   4.94495
Kieserite       MgSO4.H2O             1.783E-02     3.35278   6.30902   6.11600
Anhydrite       CaSO4                 1.026E-02     1.92896   3.57101   3.97990
Magnesite       MgCO3                 1.189E-03     0.22364   0.25641   0.28577
Indirite        Mg2B6O11.15H2O        6.858E-05     0.01290   0.09815   0.05658
Celestite       SrSO4                 9.019E-05     0.01696   0.04236   0.04721
Sellaite        MgF2                  3.262E-05     0.00613   0.00520   0.00579
   -            Li2SO4.H2O            1.441E-05     0.00271   0.00472   0.00452
Wagnerite       Mg2(PO4)F             2.105E-06     0.00040   0.00088   0.00098
Barite          BaSO4                 9.469E-08     0.00002   0.00006   0.00006
                                      ---------   --------- --------- ---------
                         Total        5.318E-01   100.00000 100.00001 100.00000

Simple salts
------------
                                        percent
                                  -------------------
                                     mole     weight

                           Na2Cl2  77.39011  78.17679
                           K2Cl2    1.68711   2.17345
                           MgCl2   11.24595   9.25615
                           CaSO4    3.39056   3.98448
                           MgSO4    5.89323   6.12305
                           MgCO3    0.39310   0.28610
                                  --------- ---------
                            Total 100.00001  99.99997
-------------------------------------------------------------------------------
NOTES: 1. Solute mole ratios calculated from initial analytical data;
          alkali/halide ratio excludes lithium and fluoride.
       2. g/kgW = grams per kilogram water.
       3. Mole percent Br in Cl sites = 0.1541; I in Cl sites = 0.000072.
Sample  1 in file: ocean         No simple-salt file created.         4-28-1986


                   SUMMARY OF REQUIRED CALCULATIONS

COMPOSITION OF SEAWATER

  1. Sea water                Riley & Chester (1971); Wedepohl (1971)
    Salt-pair tests =117667       Assemblage tests =1954       Inversions = 851
```

APPENDIX IV

Examples of SNORM Output--Standard Format

```
COMPOSITION OF SEAWATER
Riley & Chester (1971); Wedepohl (1971)                                                          Sea water
------------------------------------------------------------------------------------------------------------

Solution properties:          ph =  8.00          density = 1.030

   Water composition (analytical units: mg/kg)          Mole ratios          Concentrations adjusted to achieve charge balance
 -----------------------------------------------                             -------------------------------------------------
         molal     g/kgW      M/kg       mg/kg           Ca/Mg 1.93E-01                molal      g/kgW      M/kg       mg/kg
                                                          K/Na 2.18E-02
 Mg   5.514E-02 1.340E+00 5.320E-02 1.293E+03      Mg+Ca/Na+K 1.33E-01      Mg   5.516E-02 1.341E+00 5.322E-02 1.293E+03
 Ca   1.063E-02 4.260E-01 1.025E-02 4.110E+02       alk./hal. 8.75E-01      Ca   1.063E-02 4.261E-01 1.026E-02 4.111E+02
 Sr   9.345E-05 8.188E-03 9.016E-05 7.900E+00        HCO3/Cl 4.29E-03       Sr   9.348E-05 8.191E-03 9.019E-05 7.902E+00
 Ba   9.811E-08 1.347E-05 9.466E-08 1.300E-02         SO4/Cl 5.17E-02       Ba   9.814E-08 1.348E-05 9.469E-08 1.300E-02
 Li   2.986E-05 2.073E-04 2.881E-05 2.000E-01           F/Cl 1.23E-04       Li   2.987E-05 2.074E-04 2.882E-05 2.001E-01
 Na   4.852E-01 1.115E+01 4.681E-01 1.076E+04          Br/Cl 1.54E-03       Na   4.853E-01 1.116E+01 4.683E-01 1.077E+04
 K    1.058E-02 4.135E-01 1.021E-02 3.990E+02           I/Cl 7.22E-07       K    1.058E-02 4.137E-01 1.021E-02 3.991E+02
 F    6.983E-05 1.327E-03 6.737E-05 1.280E+00         PO4/Cl 3.86E-06       F    6.981E-05 1.326E-03 6.735E-05 1.280E+00
 Cl   5.658E-01 2.006E+01 5.459E-01 1.935E+04           B/Cl 7.54E-04       Cl   5.656E-01 2.009E+01 5.45[illegible]E-01 1.938E+04
 Br   8.729E-04 6.975E-02 8.423E-04 6.730E+01          Mg/Cl 9.75E-02       Br   8.727E-04 6.973E-02 8.4[illegible]E-04 6.727E+01
 I    4.084E-07 5.182E-05 3.940E-07 5.000E-02          Ca/Cl 1.88E-02       I    4.082E-07 5.180E-05 3.9[illegible]E-07 4.998E-02
 HCO3 2.429E-03 1.482E-01 2.344E-03 1.430E+02          Sr/Cl 1.65E-04       HCO3 2.391E-03 1.459E-01 2.30[illegible]E-03 1.408E+02
 CO3      -         -         -         -              Ba/Cl 1.73E-07       CO3  3.706E-05 2.224E-03 3.576E-05 2.146E+00
 SO4  2.923E-02 2.808E+00 2.820E-02 2.709E+03          Li/Cl 5.28E-05       SO4  2.922E-02 2.807E+00 2.819E-02 2.708E+03
 B    4.266E-04 4.612E-03 4.116E-04 4.450E+00          Na/Cl 8.58E-01       B    4.265E-04 4.611E-03 4.115E-04 4.448E+00
 PO4  2.183E-06 2.073E-04 2.106E-06 2.000E-01           K/Cl 1.87E-02       PO4  2.182E-06 2.072E-04 2.105E-06 1.999E-01
      --------- --------- --------- ---------                                    --------- --------- --------- ---------
 Total 1.160E+00 3.643E+01 1.120E+00 3.515E+04                              Total 1.160E+00 3.647E+01 1.120E+00 3.518E+04

    Charge balance:  sum[+]/sum[-] = 0.9993                         Note: borate charge of -0.667 per boron.

Normative salt assemblage                                                                      Simple salts
-------------------------                                                                      ------------
                                  per kilogram of solution      normative salts - percent                percent
                                 ---------------------------   --------------------------          -----------------
                                  moles      mg     mg (anhy)    mole     weight  wt.(anhy)             mole     weight

Halite      NaCl                4.683E-01 2.740E+04 2.740E+04  88.05749 70.06436 78.08681      Na2Cl2 77.39011 78.17679
Bischofite  MgCl2.6H2O          2.381E-02 4.845E+03 2.271E+03   4.47838 12.38930  6.47149      K2Cl2   1.68711  2.17345
Carnallite  KMgCl3.6H2O         1.021E-02 2.838E+03 1.735E+03   1.91966  7.25858  4.94495      MgCl2  11.24595  9.25615
Kieserite   MgSO4.H2O           1.783E-02 2.467E+03 2.146E+03   3.35278  6.30902  6.11600      CaSO4   3.39056  3.98448
Anhydrite   CaSO4               1.026E-02 1.396E+03 1.396E+03   1.92896  3.57101  3.97990      MgSO4   5.89323  6.12305
Magnesite   MgCO3               1.189E-03 1.003E+02 1.003E+02   0.22364  0.25641  0.28577      MgCO3   0.39310  0.28610
Indirite    Mg2B6O11.15H2O      6.858E-05 3.838E+01 1.985E+01   0.01290  0.09815  0.05658
Celestite   SrSO4               9.019E-05 1.657E+01 1.657E+01   0.01696  0.04236  0.04721
Sellaite    MgF2                3.262E-05 2.032E+00 2.032E+00   0.00613  0.00520  0.00579
   -        Li2SO4.H2O          1.441E-05 1.844E+00 1.584E+00   0.00271  0.00472  0.00452
Wagnerite   Mg2(PO4)F           2.105E-06 3.422E-01 3.422E-01   0.00040  0.00088  0.00098
Barite      BaSO4               9.469E-08 2.210E-02 2.210E-02   0.00002  0.00006  0.00006
                                --------- --------- ---------  --------- -------- ---------          --------- ---------
                      Total     5.318E-01 3.911E+04 3.509E+04 100.00000 100.00001 100.00000          100.00001 99.99997
------------------------------------------------------------------------------------------------------------
NOTES: 1. Solute mole ratios calculated from initial analytical data; alkali/halide ratio excludes lithium and fluoride.
       2. g/kgW = grams per kilogram water.
       3. Mole percent Br in Cl sites = 0.1541; I in Cl sites = 0.000072.

Sample  1 in file: ocean                      No simple-salt file created.                            4-28-1986


                    SUMMARY OF REQUIRED CALCULATIONS

COMPOSITION OF SEAWATER

  1. Sea water                Riley & Chester (1971); Wedepohl (1971)
    Salt-pair tests =117667      Assemblage tests =1954       Inversions = 851
```

Table 6. Prohibited associations in normative salt assemblages

Prohibited salt pairs

	Calcite	Dolomite	Magnesite	Trona	Pirssonite	Kalicinite	Strontionite	Witherite	Teschemacherite	Li_2CO_3	Anhydrite	Kieserite	Thenardite	Arcanite	Glauberite	Syngenite	Polyhalite	Bloedite	Leonite	Aphthitalite	Celestite	Barite	Mascagnite	$Li_2SO_4\cdot H_2O$	Burkeite	Antarcticite	Tachyhydrite	Bischofite	Carnallite	Sylvite	Halite	$SrCl_2\cdot 2H_2O$	$BaCl_2\cdot H_2O$	Salammoniac	$LiCl\cdot H_2O$	Kainite	Nitrocalcite	Nitromagnesite	Niter	Soda niter	$Sr(NO_3)_2$	Nitrobarite	Ammonia niter	$LiNO_3\cdot 3H_2O$	Inyoite	Ulexite	Indirite	Borax	Fluorite	Sellaite	Villiaumite	LiF	Hydroxyapatite	$Mg_3(PO_4)_2$	Na_3PO_4	Fluorapatite
Dolomite																																																								
Magnesite	X																																																							
Trona	X																																																							
Pirssonite			X																																																					
Kalicinite																																																								
Strontionite																																																								
Witherite																																																								
Teschemacherite																																																								
Li_2CO_3																																																								
Anhydrite*				X	X	X	X	X	X	X																																													
Kieserite*	X	X		X	X	X	X	X	X	X																																													
Thenardite*				X		X		X	X	X	X	X																																											
Arcanite											X	X	X																																											
Glauberite				X	X	X	X	X	X	X		X		X																																									
Syngenite				X	X	X	X	X	X	X		X	X																																										
Polyhalite	X	X		X	X	X	X	X	X	X			X	X																																									
Bloedite	X	X		X	X	X	X	X	X	X				X																																									
Leonite*	X	X		X	X	X	X	X	X	X	X		X		X																																								
Aphthitalite						X		X	X	X	X	X																																												
Celestite				X	X	X		X	X																																															
Barite						X			X																																																
Mascagnite						X		X																																																	
$Li_2SO_4\cdot H_2O$						X		X	X																																															
Burkeite	X					X		X	X	X	X	X	X	X	X	X	X	X	X		X		X																																	
Antarcticite			X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X																															
Tachyhydrite	X		X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X																															
Bischofite	X			X	X	X	X	X	X	X			X	X	X	X	X	X	X	X			X		X	X																														
Carnallite				X	X	X			X				X	X	X	X		X	X	X			X		X																															
Sylvite												X	X		X			X					X		X		X	X																												
Halite						X			X					X									X																																	
$SrCl_2\cdot 2H_2O$*				X	X	X		X	X			X	X	X	X	X	X	X	X	X			X		X																															
$BaCl_2\cdot H_2O$*				X	X	X			X			X	X	X	X	X	X	X	X	X	X		X	X	X																															
Salammoniac						X																																																		
$LiCl\cdot H_2O$				X	X	X	X	X	X			X	X	X	X	X	X	X	X	X	X		X		X																															
Kainite	X	X		X	X	X	X	X	X	X	X		X	X	X	X		X		X			X		X	X	X	X				X	X		X																					
Nitrocalcite				X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X							X	X			X																				
Nitromagnesite	X	X		X	X	X	X	X	X	X			X	X	X	X	X	X	X	X			X		X	X	X			X		X	X		X	X																				
Niter																										X	X	X				X	X		X																					
Soda niter						X			X					X		X	X		X	X			X			X	X	X		X		X	X		X	X																				
$Sr(NO_3)_2$				X	X	X		X	X			X	X	X	X	X	X	X	X	X			X		X								X			X																				
Nitrobarite				X	X	X			X			X	X	X	X	X	X	X	X	X	X		X		X											X																				
Ammonia niter						X								X												X	X	X	X	X	X	X	X		X	X																				
$LiNO_3\cdot 3H_2O$				X	X	X	X	X	X			X	X	X	X	X	X	X	X	X	X	X	X		X	X	X					X	X			X																				
Inyoite				X	X							X	X	X	X	X	X	X	X	X					X											X																				
Ulexite				X	X							X	X							X					X	X	X	X	X							X	X	X																		
Indirite	X	X		X	X								X		X	X				X					X	X	X										X																			
Borax											X	X														X	X	X	X							X	X	X							X											
Fluorite				X	X							X					X	X	X						X											X		X																		
Sellaite	X	X		X	X																				X	X	X										X								X	X										
Villiaumite										X	X	X			X	X	X	X	X					X		X	X	X	X						X	X	X	X						X	X	X	X									
LiF											X	X			X	X	X	X	X							X	X	X	X							X	X	X																		
Hydroxyapatite												X					X	X	X																	X													X	X	X	X				
$Mg_3(PO_4)_2$	X	X			X																					X	X										X								X				X	X	X	X				
Na_3PO_4	X	X	X		X						X	X			X	X	X	X	X							X	X	X	X							X	X	X							X	X	X		X	X						
Fluorapatite												X					X	X	X																	X																		X		
Wagnerite	X	X			X																					X	X										X								X				X							

Prohibited three-phase salt associations

Bloedite-syngenite-anhydrite
Leonite-bloedite-syngenite
Aphthitalite-polyhalite-glauberite
Bischofite-celestite-dolomite
Carnallite-celestite-calcite

Sylvite-antarcticite-dolomite
Halite-picromerite-syngenite
$BaCl_2\cdot H_2O$-anhydrite-magnesite
Nitrocalcite-sylvite-magnesite
Niter-carnallite-calcite

Niter-nitromagnesite-halite
Soda niter-carnallite-dolomite
Soda niter-carnallite-calcite
Ulexite-$(Sr/Ba)(Cl/NO_3)_2\cdot nH_2O$-anhydrite
Indirite-$(Sr/Ba)(Cl/NO_3)_2\cdot nH_2O$-anhydrite

Borax-polyhalite-glauberite
Sellaite-$(Sr/Ba)(Cl/NO_3)_2\cdot nH_2O$-anhydrite
$Mg_3(PO_4)_2$-$(Sr/Ba)(Cl/NO_3)_2\cdot nH_2O$-anhydrite
Wagnerite-$(Sr/Ba)(Cl/NO_3)_2\cdot nH_2O$-anhydrite

Prohibited four-phase salt associations

$SrCl_2\cdot 2H_2O$-sylvite-anhydrite-magnesite
$BaCl_2\cdot H_2O$-sylvite-anhydrite-dolomite
$Sr(NO_3)_2$-carnallite-barite-calcite
Nitrobarite-sylvite-anhydrite-magnesite

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*Higher hydration states, gypsum, epsomite, mirabilite, picromerite, $SrCl_2\cdot 6H_2O$, $BaCl_2\cdot 2H_2O$, respectively, may replace these phases.

Table II-5. Prohibited "base salt" associations in SNORM's "base-salt assemblages"

[Salt numbers refer to table II-3]

Prohibited salt pairs	1. Calcite	2. Dolomite	3. Magnesite	4. Na_2CO_3*	5. Pirssonite	6. K_2CO_3*	7. Strontionite	8. Witherite	9. $(NH_4)_2CO_3$*	10. Li_2CO_3	11. Anhydrite	12. Kieserite	13. Thenardite	14. Arcanite	15. Glauberite	16. Syngenite	17. Polyhalite	18. Bloedite	19. Leonite	20. Aphthitalite	21. Celestite	22. Barite	23. Mascagnite	24. $Li_2SO_4 \cdot H_2O$	25. Antarcticite	26. Tachyhydrite	27. Bischofite	28. Carnallite	29. Sylvite	30. Halite	31. $SrCl_2 \cdot 2H_2O$	32. $BaCl_2 \cdot H_2O$	33. Salammoniac	34. $LiCl \cdot H_2O$	35. Nitrocalcite	36. Nitromagnesite	37. Niter	38. Soda niter	39. $Sr(NO_3)_2$	40. Nitrobarite	41. Ammonia niter	42. $LiNO_3 \cdot 3H_2O$	43. Inyoite	44. Ulexite	45. Indirite	46. Borax	47. Fluorite	48. Sellaite	49. Villiaumite	50. LiF	51. $Ca_3(PO_4)_2$*	52. $Mg_3(PO_4)_2$	53. Na_3PO_4	54. Fluorapatite
2. Dolomite																																																						
3. Magnesite	X																																																				
4. Na_2CO_3*	X																																																				
5. Pirssonite			X																																																		
6. K_2CO_3*																																																						
7. Strontionite																																																						
8. Witherite																																																						
9. $(NH_4)_2CO_3$*																																																						
10. Li_2CO_3																																																						
11. Anhydrite				X	X	X	X	X	X	X																																												
12. Kieserite	X	X		X	X	X	X	X	X	X																																												
13. Thenardite						X		X	X	X	X	X																																										
14. Arcanite											X	X	X																																										
15. Glauberite				X	X	X	X	X	X	X		X		X																																								
16. Syngenite				X	X	X	X	X	X	X		X	X																																									
17. Polyhalite	X	X		X	X	X	X	X	X	X			X	X																																								
18. Bloedite	X	X		X	X	X	X	X	X	X				X																																								
19. Leonite	X	X		X	X	X	X	X	X	X	X		X		X																																							
20. Aphthitalite						X		X	X	X	X	X																																										
21. Celestite				X	X	X		X	X																																													
22. Barite						X			X																																													
23. Mascagnite				X	X	X		X																																														
24. $Li_2SO_4 \cdot H_2O$								X	X																																													
25. Antarcticite			X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X																														
26. Tachyhydrite	X		X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X																														
27. Bischofite	X			X	X	X	X	X	X	X			X	X	X	X	X	X	X	X			X		X																												
28. Carnallite				X	X	X			X				X	X	X	X		X	X	X			X																														
29. Sylvite													X		X			X					X			X	X																											
30. Halite						X			X					X									X																														
31. $SrCl_2 \cdot 2H_2O$				X	X	X		X	X			X	X	X	X	X	X	X	X	X			X																														
32. $BaCl_2 \cdot H_2O$				X	X	X			X			X	X	X	X	X	X	X	X	X	X		X	X																													
33. Salammoniac						X																																																
34. $LiCl \cdot H_2O$				X	X	X	X	X	X			X	X	X	X	X	X	X	X	X	X		X																														
35. Nitrocalcite				X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X							X	X																					
36. Nitromagnesite	X	X		X	X	X	X	X	X	X			X	X	X	X	X	X	X	X			X		X	X			X		X	X		X																					
37. Niter																									X	X	X				X	X		X																					
38. Soda niter						X			X					X		X	X		X	X			X		X	X	X		X		X	X		X																					
39. $Sr(NO_3)_2$				X	X	X		X	X			X	X	X	X	X	X	X	X	X			X									X																							
40. Nitrobarite				X	X	X			X			X	X	X	X	X	X	X	X	X	X		X																														
41. Ammonia niter						X								X											X	X	X	X	X	X	X	X		X																					
42. $LiNO_3 \cdot 3H_2O$				X	X	X	X	X	X			X	X	X	X	X	X	X	X	X	X	X	X		X	X					X	X																							
43. Inyoite				X	X							X	X	X	X	X	X	X	X	X																																		
44. Ulexite				X	X							X	X							X					X	X	X	X							X	X																			
45. Indirite	X	X		X	X								X		X	X				X					X	X									X																					
46. Borax											X	X													X	X	X	X							X	X							X											
47. Fluorite				X	X							X					X	X	X																		X																		
48. Sellaite	X	X		X	X																			X	X									X							X	X										
49. Villiaumite										X	X	X			X	X	X	X	X					X	X	X	X	X							X	X	X						X	X	X	X									
50. LiF											X	X			X	X	X	X	X							X	X	X	X							X	X																		
51. $Ca_3(PO_4)_2$*												X					X	X	X																													X	X	X	X				
52. $Mg_3(PO_4)_2$	X	X			X																					X	X									X							X				X	X	X	X				
53. Na_3PO_4	X	X	X		X						X	X			X	X	X	X	X							X	X	X	X							X	X							X	X	X		X	X						
54. Fluorapatite												X					X	X	X																																		X		
55. Wagnerite	X	X			X																					X	X									X							X				X								

Prohibited three-phase salt associations

Bloedite-syngenite-anhydrite
Leonite-bloedite-syngenite
Aphthitalite-polyhalite-glauberite
Bischofite-celestite-dolomite
Carnallite-celestite-calcite

Sylvite-kieserite-anhydrite
Sylvite-antarcticite-dolomite
Halite-picromerite-syngenite
$BaCl_2 \cdot H_2O$-anhydrite-magnesite
Nitrocalcite-sylvite-magnesite

Niter-carnallite-calcite
Niter-nitromagnesite-halite
Soda niter-carnallite-dolomite
Soda niter-carnallite-calcite
Ulexite-$(Sr/Ba)(Cl/NO_3)_2 \cdot nH_2O$-anhydrite

Indirite-$(Sr/Ba)(Cl/NO_3)_2 \cdot nH_2O$-anhydrite
Borax-polyhalite-glauberite
Sellaite-$(Sr/Ba)(Cl/NO_3)_2 \cdot nH_2O$-anhydrite
$Mg_3(PO_4)_2$-$(Sr/Ba)(Cl/NO_3)_2 \cdot nH_2O$-anhydrite
Wagnerite-$(Sr/Ba)(Cl/NO_3)_2 \cdot nH_2O$-anhydrite

Prohibited four-phase salt associations

$SrCl_2 \cdot 2H_2O$-sylvite-anhydrite-magnesite
$BaCl_2 \cdot H_2O$-sylvite-anhydrite-dolomite
$Sr(NO_3)_2$-carnallite-barite-calcite
Nitrobarite-sylvite-anhydrite-magnesite

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* Not normative salts; used to expedite caluclations; replaced by trona, kalicinite, teschemacherite, and hydroxyapatie in norm.