Canadian Mineralogist
Vol. 19, pp. 441-450 (1981)

THE GLADSTONE-DALE RELATIONSHIP: PART IV. THE COMPATIBILITY CONCEPT AND ITS APPLICATION

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ABSTRACT

The compatibility index ($1 - K_P/K_C$), applied to 834 sets of data from Winchell & Winchell (1964), characterizes 406 sets (49%) as superior, 179 (21%) as excellent, 93 (11%) as good, 39 (5%) as fair and 117 (14%) as poor. Revised constants are proposed for WO_3 (0.171), P_2O_5 (0.183), SeO_2 (0.195), TeO_2 (0.201) and TeO_3 (0.172). Constants are presented for twelve organic constituents as well as for SO (0.335), PdO (0.190), PtO (0.118), PO_2 (0.236), PtO_2 (0.151) and Re_2O_7 (0.130). Among the organic constituents, C_2O_3 has its value revised from 0.270 to 0.267. Additional constants to be used only for neso- and inosilicates are Al_2O_3 (0.176), Ti_2O_3 (0.227), V_2O_3 (0.237), Cr_2O_3 (0.247) and Mn_2O_3 (0.256). Application of the compatibility index to other sets of data (garnets, axinites, scapolites and new minerals) allows assessment of the data and commonly points out errors. Individual k values should be called Gladstone–Dale constants, not specific refractive energies.

Keywords: Gladstone–Dale constants, compatibility index, synthetic compounds, silicates, new species, organic, inorganic.

SOMMAIRE

L'index de compatibilité ($1 - K_P/K_C$) a été calculé pour 834 groupes de données tirées de Winchell & Winchell (1964); 406 de ceux-ci (49%) s'avèrent supérieurs, 179 (21%) excellents, 93 (11%) bons, 39 (5%) passables et 117 (14%) piètres. On propose des constantes révisées pour WO_3 (0.171), P_2O_5 (0.183), SeO_2 (0.195), TeO_2 (0.201) et TeO_3 (0.172). On présente des constantes pour douze composants organiques ainsi que pour SO (0.335), PdO (0.190), PtO (0.118), PO_2 (0.236), PtO_2 (0.151) et Re_2O_7 (0.130). Pour un des composants organiques, C_2O_3, la valeur de la constante passe de 0.270 à 0.267. Des constantes à utiliser pour nésosilicates et inosilicates sont les suivantes: Al_2O_3 (0.176), Ti_2O_3 (0.227), V_2O_3 (0.237), Cr_2O_3 (0.247) et Mn_2O_3 (0.256). L'application de l'indice de compatibilité à d'autres ensembles de données (grenats, axinites, scapolites, minéraux nouveaux) permet l'évaluation des données et, dans plusieurs cas, le dépistage d'erreurs. Les valeurs individuelles de k devraient s'appeler constantes de Gladstone–Dale et non pas "énergies réfractives spécifiques".

(Traduit par la Rédaction)

Mots-clés: constantes de Gladstone–Dale, indice de comptabilité, composés synthétiques, silicates, minéraux nouveaux, organique, inorganique.

INTRODUCTION

In Part III of this series, and using $K_P = (\bar{n}-1)/D$ and $K_C = k_1p_1/100 + k_2p_2/100... + k_np_n/100$, Mandarino (1979) proposed that the quantity ($1 - K_P/K_C$) be used as a measure of the compatibility of the mean index of refraction, density and chemical composition. This quantity, henceforth called the *compatibility index*, was used to set up a scale by which the internal consistency of data for a compound could be characterized by certain adjectives. The scale proposed is:

Compatibility Index	*Category*
±0.000 to ±0.019	Superior
±0.020 to ±0.039	Excellent
±0.040 to ±0.059	Good
±0.060 to ±0.079	Fair
> ±0.079	Poor

The limits for these categories were selected quite arbitrarily; a few words are in order to explain what they represent in terms of actual values of the mean index of refraction and density. In each of the following examples, it is assumed that the value of K_C is correct. In other words, the chemical formula and the individual k values used for the constituents are assumed correct. Therefore, any deviation of K_P/K_C from unity is due to an error in K_P which, in turn, is caused by errors in $\bar{n}$ or D (or both). For a compound with $K_C = 0.200$, $\bar{n} = 1.600$ and $D = 3.000$ g/cm^3, the data will fall into the superior category if the errors in $\bar{n}$ and D do not exceed ±0.002 and ±0.070, respectively. A compound with $K_C = 0.300$, $\bar{n} = 1.600$ and $D = 2.000$ g/cm^3 will have data that fall into the superior category if the errors in $\bar{n}$ and D are less than ±0.002 and ±0.047, respectively.

TEST OF THE CONCEPT OF A COMPATIBILITY INDEX

To test the concept of a compatibility index, it was decided to carry out calculations with data from a large number of compounds. The compilation of Winchell & Winchell (1964) provided data for numerous synthetic compounds; this selection should keep errors in chemical composition to a minimum. The sole criterion for selection of a particular compound was the completeness of the appropriate data (*i.e.*, chemical formula, indices of refraction and density). In a few instances, compounds known to be of doubtful validity were rejected. Data from 834 compounds were used to calculate K_C, K_P and $1 - K_P/K_C$. Table 1 shows that this resulted in 406 sets of data (49%) being characterized as superior, 179 (21%) as excellent, 93 (11%) as good, 39 (5%) as fair and 117 (14%) as poor.

Because data for synthetic compounds were used to minimize errors in chemical composition, large values of $1 - K_P/K_C$ are probably due to errors in $\bar{n}$ or D (or both). Although one should not discount the possibility of errors in individual values of k, the overwhelmingly large percentage (81%) of compounds falling within the superior, excellent and good categories tends to support the concept of the compatibility index.

An attempt was made to check the data for the 117 compounds that were placed in the Poor category. Data for 85 of these compounds were found in the compilation of Donnay & Ondik (1973). Of these, 12 showed no significant changes, two had different chemical compositions, one had new optical data, 68 had new density data and two had all three sets of data different from those given earlier. In addition, three of the compounds not listed by Donnay & Ondik (1973) have densities that are obviously incorrect. Comparison of the densities given by Winchell & Winchell (1964) with densities of related compounds shows unreasonable discrepancies. Indeed, two of these may be typographical errors (*i.e.*, 3.80 g/cm^3 instead of 2.80 g/cm^3). Among the 68 sets of new density data, several "new" densities are really corrections of typographical errors.

TABLE 1. DISTRIBUTION OF THE COMPATIBILITY INDEX FOR THE 834 COMPOUNDS FROM WINCHELL & WINCHELL(1964)

Compatibility category	A		B	
	N	%	N	%
Superior	406	49	413	50
Excellent	179	21	187	22
Good	93	11	99	12
Fair	39	5	44	5
Poor	117	14	91	11
Totals	834	100	834	100

A original data; B revised data from Donnay & Ondik (1973).

The 73 sets of revised data were used to recalculate values of $1 - K_P/K_C$, with the following results: seven compounds are now in the superior category, eight are excellent, six are good, five are fair and 47 remain in the poor category. The revised data are compared with the original data in Table 1. It should be emphasized that of the 91 compounds that remain in the poor category, no data are given by Donnay & Ondik (1973) in 32 cases, the data for 12 compounds were unchanged and the data for 47 did not result in reclassification. The latter remain in the poor category; even so, the recalculated $1 - K_P/K_C$ values were better for 35 and worse for 12.

COMPARISON OF THE CONCEPT AMONG DIFFERENT CHEMICAL CLASSES

The 834 compounds discussed in the preceding section include most of the chemical classes found in minerals as well as some others. The results of the calculations by chemical class (Table 2) indicate that the silica glasses, selenates, halates, sulfates, silicates and nitrates

TABLE 2. COMPATIBILITY INDEX DISTRIBUTION OF REVISED WINCHELL & WINCHELL (1964) DATA FOR VARIOUS CHEMICAL CLASSES

Chemical Class	Number						Percentage					
	S	E	G	F	P	Σ	S	E	G	F	P	Σ
silica glasses	53	4	2	0	1	60	88	7	3	0	2	100
selenates	14	0	2	0	1	17	82	0	12	0	6	100
halates	25	6	1	2	0	34	73	18	3	6	0	100
sulfates	78	31	7	5	9	130	60	24	5	4	7	100
silicates	93	34	21	6	3	157	59	22	13	4	2	100
nitrates	12	6	1	1	1	21	57	28	5	5	5	100
carbonates	23	14	8	2	2	49	47	29	16	4	4	100
borates	10	9	3	0	1	23	44	39	13	0	4	100
arsenates	13	7	5	1	4	30	44	23	17	3	13	100
phosphates	25	19	11	6	8	69	36	27	16	9	12	100
vanadates	1	0	0	0	2	3	33	0	0	0	67	100
halides	40	32	19	11	22	124	32	26	15	9	18	100
molybdates	2	1	1	0	3	7	29	14	14	0	43	100
chromates	1	2	0	0	1	4	25	50	0	0	25	100
oxides	23	22	15	8	32	100	23	22	15	8	32	100
tungstates	0	0	3	2	1	6	0	0	50	33	17	100
ALL	413	187	99	44	91	834	50	22	12	5	11	100

S = Superior, E = Excellent, G = Good, F = Fair, P = Poor all have over 50% of their data in the superior category. The carbonates fall just short of this, with 47% of their data classed as superior. The percentage of data classed as superior drops in the other classes from 44% in the borates to 0% in the tungstates.

The chemical classes were further investigated to determine whether 1) better constants for the particular anionic components could be calculated and 2) application of these constants would change the overall distribution among the categories. Results of such calculations show that most of these new constants are very close to those given by Mandarino (1976), and only the constant for WO_3 is significantly different. It is suggested that the new value for WO_3 of 0.171 should replace 0.152 given by Mandarino (1976). The new phosphate constant is 0.183, but the frequency distribution of the calculated values of k for P_2O_5 indicates two "peak" concentrations at about 0.175 and 0.190, which are close to the values given, respectively, by Mandarino (1976) and Larsen (1921). Attempts to correlate the two constants with specific kinds of phosphates (*i.e.*, "normal" *versus* "acid", hydrous *versus* anhydrous) failed. Although the application of the new constant to the phosphates of Winchell & Winchell (1964) results in only a slight change of distribution among the categories, it is suggested that this value of 0.183 be used in place of 0.176 given by Mandarino (1976). Trzcienski *et al.* (1974) derived a constant equal to 0.170 for P_2O_5 from a fluorapatite. However, they did not actually derive it from the data that they presented. If they had, the value would be 0.166 based on their measured density, or 0.184 on their calculated density. In fact, because of some errors in their calculated formula, their molecular weight and density are incorrect. If the correct calculated density is used, k for P_2O_5 is 0.179. If their data and the constants proposed by Mandarino (1976) are used, the k values of P_2O_5 from D(meas.) and D(calc.) are, respectively, 0.188 and 0.200. Using k (P_2O_5) as 0.183, the data of Trzcienski *et al.* (1974) fall into the superior category if D (meas.) is used and into the excellent category if D(calc.) is used.

Oxides

The 100 sets of data for oxides given by Winchell & Winchell (1964) enabled oxide constants to be calculated for 35 oxide constituents. Some of these were calculated from simple oxides (*i.e.*, the oxide of a single cation, such as MgO), others were calculated from multiple oxides (*i.e.*, the oxide of more than one cation, such as $MgAl_2O_4$), and still others were calculated from both kinds of oxides. Table 3 gives the results of these calculations and compares the new "oxide" constants with the general constants proposed by Mandarino (1976). Over a third of the oxide constants are identical or very close to Mandarino's general constants (*i.e.*, within ±5%). There does not seem to be any clear relationship between the general constants and the corresponding oxide constants. Therefore, it does not seem reasonable to suggest that any of these oxide constants should be used when working with oxides. This is particularly true in that many of the oxide constants were calculated from very few sets of data, and thus are more likely to contain significant errors. On the other hand, use of these oxide constants in the calculation of $1 - K_P/K_C$ dramatically changes the distribution among the categories. The largest changes are in the superior category (from 23 to 41%) and in the poor category (from 29 to 10%). Ten of the oxide constants were calculated from single sets of data and, among these, seven were simple oxides. Consequently, the value of

TABLE 3. CONSTANTS CALCULATED FROM OXIDES

Constituent	Regular k Mandarino (1976)	Oxide k	% Difference from Regular k to Oxide k
H_2O	0.340	0.335	-1.5
Li_2O	0.307	0.312	1.6
Na_2O	0.190	0.232	22.1
* Cu_2O	0.234	0.277	18.4
BeO	0.240	0.222	-7.5
MgO	0.200	0.197	-1.5
CaO	0.210	0.233	11.0
MnO	0.197	0.215	9.1
FeO	0.188	0.192	2.1
* NiO	0.176	0.186	5.7
CuO	0.170	0.204	20.0
ZnO	0.158	0.125	-20.9
SrO	0.145	0.163	12.4
CdO	0.130	0.164	26.2
BaO	0.128	0.148	15.6
* HgO	0.123	0.135	9.8
PbO	0.133	0.168	26.3
B_2O_3	0.215	0.241	12.1
Al_2O_3	0.207	0.195	-5.8
Cr_2O_3	0.290	0.220	-24.1
Mn_2O_3	0.301	0.304	1.0
Fe_2O_3	0.315	0.317	0.6
Ga_2O_3	0.170	0.104	-38.8
As_2O_3	0.235	0.210	-10.6
Sb_2O_3	0.203	0.210	3.4
SiO_2	0.208	0.207	-0.5
TiO_2	0.393	0.379	-3.6
GeO_2	0.167	0.166	-0.6
* ZrO_2	0.211	0.209	-0.9
* SnO_2	0.143	0.148	3.5
* TeO_2	0.183	0.200	9.3
* ThO_2	0.167	0.124	-25.7
P_2O_5	0.176	0.207	17.6
WO_3	0.152	0.157	3.3
UO_3	0.118	0.126	6.8

*These oxides are those for which constants were calculated from a single simple oxide (*i.e.* the oxide k is the K_p of the oxide.)

K_P is automatically equal to K_C for these compounds, the value of $1 - K_P/K_C$ is zero, and the data are placed in the superior category. If these seven sets of data are deleted from the distribution, there is still a substantial change in the superior category (from 23 to 36%) and in the poor category (from 29 to 11%). With constants for only 35 constituents, it is doubtful whether these oxide constants will be of much use. Also, since many oxides are opaque, the Gladstone–Dale relationship is not applicable; many others have such high indices of refraction that large errors of measurement may be present, adversely affecting the application of the Gladstone–Dale relationship to these oxides.

Until a major study of a large number of reliable sets of data for a wide selection of oxides becomes available, we must face the unsatisfactory conclusion that the Gladstone–Dale relationship is not applicable to all oxides.

Silicates

Special additional attention was given to silicates becauses they represent the single largest chemical class among minerals (about 25%) and because for many years the author has been aware of the nonconformance of certain silicates with regard to the Gladstone–Dale relationship. The most notable example of silicates that do not conform to the relationship is the garnet group, discussed in a later section.

Deer *et al.* (1962a, b, c, 1963) provided 505 sets of data for which values of K_P and K_C can be calculated. The distribution of the compatibility indices ($1 - K_P/K_C$) for these data is given in Table 4, where a comparison is made with the revised results for the silicates from Winchell & Winchell (1964). It is apparent that more of the data from Deer *et al.* fall into the superior compatibility category than do the data from Winchell & Winchell (1964). This is probably due to the fact that calculations of K_C for the compounds given by Winchell & Winchell (1964) were carried out for the ideal formulae given by them, although the compounds are probably not that pure. On the other hand, the values of K_C for the minerals given by Deer *et al.* (1962a, b, c, 1963) were calculated from actual analyses. Table 5 shows the distribution of the data from Deer *et al.* among the specific types of silicate structure; it is clear that the nesosilicates and phyllosilicates have far fewer sets of data in the superior category than do the other types of silicates. Much of the poor compatibility among the phyllosilicates probably results from poor physical data. It is commonly extremely difficult to measure all the principal indices of refraction of the many micaceous species.

TABLE 4. DISTRIBUTION OF $1\text{-}K_p/K_C$ FOR SILICATES

Category	505 silicates from Deer *et al.* (1962*a*, *b*, *c*, 1963)	157 silicates from Winchell & Winchell (1964)
Superior	70%	59%
Excellent	21	22
Good	7	13
Fair	1	4
Poor	1	2
Total	100	100

Since it is more difficult to understand the results among the nesosilicates, they were examined more carefully. One of the first observations made was that minerals with high amounts of Fe_2O_3 *generally* show better compatibility than do minerals with high amounts of Al_2O_3. When the new constants given by Mandarino (1976) were first derived, it was found that certain compounds gave a k value for Fe_2O_3 of 0.315 whereas silicates gave a value of 0.268. Jaffe (1956) gave the values of 0.310 for Fe_2O_3 in hydrated sulfates and 0.290 in silicates. In the present study, the author theorized that special constants were needed for the other trivalent constituents in silicates; thus new k values for Al_2O_3, V_2O_3, Cr_2O_3 and Mn_2O_3 were derived by multiplying the old constants by 0.851, which is the ratio of the "silicate" Fe_2O_3 constant (0.268) to the other Fe_2O_3 constant (0.315). The "silicate" constants derived in this way are: Al_2O_3 0.176, Ti_2O_3 0.227, V_2O_3 0.237, Cr_2O_3 0.247, Mn_2O_3 0.256 and Fe_2O_3 0.268.

Values of K_C and of the compatibility index were recalculated for each of the 505 sets of data given by Deer *et al.* (1962a, b, c, 1963) using the foregoing trivalent constants. The percentages in the various categories are: Superior 48(70), Excellent 33(21), Good 13(7), Fair 5(1) and Poor 1(1). The figures in brackets are the percentages from Table 4 using the constants given by Mandarino (1976). It ap-

TABLE 5. DISTRIBUTION OF $1\text{-}K_p/K_C$ AMONG SILICATE STRUCTURE-TYPES*

Silicate structure-type	Category superior	excellent	good	fair	poor
Nesosilicates	40%	39%	20%	1%	0%
Sorosilicates	81	16	3	0	0
Cyclosilicates	78	18	2	0	2
Inosilicates	72	20	6	1	1
Phyllosilicates	55	26	11	4	4
Tectosilicates	91	9	0	0	0

*Data from Deer *et al.* (1962*a*, *b*, *c*, 1963).

pears that the new trivalent constants give poorer results than did the old constants. However, if the results in the various structure types are examined, a different picture evolves. Table 6 lists, by silicate structure type, the distribution of values of the compatibility index determined from K_C values that were calculated using three sets of k values. Those marked M were calculated using the constants given by Mandarino (1976). Those marked MR represent those calculated with the same constants except that the revised constants for the trivalent constituents were used. For further comparison, data are included for calculations carried out with the constants given by Larsen (1921) and revised by Jaffe (1956); these are marked L&J. For each structure type, the highest percentage in the superior category is italicized. The highest percentage of superior data in the nesosilicates is the result of calculations using the revised (MR) constants. The same is true of the inosilicates, although there the difference between the results from the revised constants (MR) and the original constants (M) may not be significant. In all the other structure types (sorosilicates, cyclosilicates, phyllosilicates and tectosilicates), the results obtained from the original Mandarino constants give the highest percentages in the superior category. In the tectosilicates, however, there may not be a significant difference between the results using the Larsen–Jaffe constants and those using the Mandarino constants.

It is recommended that the revised constants for the trivalent constituents be used for only the nesosilicates and inosilicates; the constants given by Mandarino (1976) should be used for all other silicates. That the Mandarino constants place more of the data from Deer *et al.* (1962a, b, c, 1963) in the superior category than do the Larsen–Jaffe constants is evident from Table 6.

COMPARISON OF MANDARINO CONSTANTS AND LARSEN–JAFFE CONSTANTS

The superiority of the constants proposed by the author over those proposed by Larsen and revised by Jaffe has already been demonstrated for the silicates (Table 6). For the data taken from Deer *et al.* (1962a, b, c, 1963), 73.5% fall into the superior category using Mandarino's constants compared with 51.3% using the Larsen–Jaffe constants. Similar results were found for the silicate data given by Winchell & Winchell (1964): the Mandarino constants placed 74.1% of the data in the superior category compared with 57.9% for the Larsen–Jaffe constants. For nonsilicates the differences are not so striking; the use of either set of constants gives similar statistical results. For the 834 sets of data from Winchell & Winchell (1964) the Mandarino constants give a slightly better distribution among the various categories than do the Larsen–Jaffe constants.

One of the main advantages of using the Mandarino constants instead of the Larsen–Jaffe constants is the greater number of constituents covered by the former.

NEW CONSTANTS AND THE RELIABILITY OF CONSTANTS

During the course of this entire study, numerous constants for the Gladstone–Dale re-

TABLE 6. DISTRIBUTION OF THE COMPATIBILITY INDEX AMONG THE SILICATE STRUCTURE-TYPES FOR DATA TAKEN FROM DEER *ET AL.**

Silicate Structure-type	Compatibility Category	(L & J)	(M)	(MR)
	S	30	40	*54*
	E	28	39	30
Nesosilicates	G	29	20	11
	F	12	1	4
	P	1	0	1
		100	100	100
	S	16	*81*	24
	E	52	16	55
Sorosilicates	G	32	3	16
	F	0	0	5
	P	0	0	0
		100	100	100
	S	45	*78*	20
	E	45	18	50
Cyclosilicates	G	8	2	25
	F	0	0	5
	P	2	2	0
		100	100	100
	S	51	72	*76*
	E	34	20	20
Inosilicates	G	12	6	3
	F	2	1	1
	P	1	1	0
		100	100	100
	S	38	*55*	43
	E	41	26	38
Phyllosilicates	G	11	11	6
	F	6	4	9
	P	4	4	4
		100	100	100
	S	88	*91*	25
	E	11	9	40
Tectosilicates	G	1	0	26
	F	0	0	9
	P	0	0	0
		100	100	100

K_C values calculated from: Larsen's constants as revised by Jaffe (L & J), Mandarino's constants (M), and Mandarino's revised constants (MR). Italicized numbers represent the highest percentages of data in the superior category for each structure-type. * Deer *et al.* (1962*a*, *b*, *c*, 1963).

lationship have been derived; 119 constants for 114 constituents were published by Mandarino (1976, 1978). Several other constants, derived from data not previously available, are included in Table 7 along with the constants previously proposed by the author. Revised constants are given for SeO_2, TeO_2 and TeO_3; information concerning these constants will appear in a paper being prepared by the author. It is suggested that the constants in Table 7 should replace all former constants.

The reliability of a *k* value for a particular constituent depends on several factors. The first of these, and the most obvious, is the accuracy of the physical data (indices of refraction and density) for the compounds used to derive the constant. Because of the empirical nature of the Gladstone–Dale relationship, the reliabilities of the constants also depend on the number of compounds used to derive them and the consequent statistical spread in the values for a

TABLE 7. REVISED GLADSTONE-DALE CONSTANTS

Component	Atomic Number	Molecular Weight	*k*	Remarks	Reliability Indicator
H_2O	1	18.02	0.340		H
Li_2O	3	29.88	0.307		H
$(NH_4)_2O$	—	52.08	0.483		H
Na_2O	11	61.98	0.190		H
K_2O	19	94.20	0.196		H
Cu_2O	29	143.09	0.234		M
Rb_2O	37	186.94	0.128		H
Ag_2O	47	231.74	0.168		M
Cs_2O	55	281.81	0.119		H
Au_2O	79	409.94	(0.152)		?
Hg_2O	80	417.18	0.144		L
			(0.134)		?
Tl_2O	81	424.74	0.115		M - H
Fr_2O	87	462	(0.115)		?
BeO	4	25.01	0.240		H
MgO	12	40.30	0.200		H
			0.225	sulfates & selenates	H
SO	16	48.06	0.335		M
CaO	20	56.08	0.210		H
VO	23	66.94	(0.207)		H
CrO	24	68.00	(0.202)		H
MnO	25	70.94	0.197		H
FeO	26	71.85	0.188		H
CoO	27	74.93	0.179		H
NiO	28	74.71	0.176		H
CuO	29	79.55	0.170		H
ZnO	30	81.37	0.158		H
SrO	38	103.62	0.145		H
PdO	46	122.40	0.190		L
CdO	48	128.40	0.130		H
SnO	50	134.69	(0.140)		?
BaO	56	153.34	0.128		H
PtO	78	211.09	0.118		L
HgO	80	216.59	0.123		M
PbO	82	223.19	0.133		M
RaO	88	242.00	(0.120)		?
B_2O_3	5	69.62	0.215		H
C_2O_3	6	72.02	0.267		H
N_2O_3	7	76.01	(0.325)		?
Al_2O_3	13	101.96	0.207		H
			0.242	sulfates & selenates	H
			0.176	nesosilicates & inosilicates	H
P_2O_3	15	109.95	(0.315)		?
Sc_2O_3	21	137.91	0.257		H
Ti_2O_3	22	143.80	(0.267)		H
			(0.227)	nesosilicates & inosilicates	H
V_2O_3	23	149.88	(0.279)		H
			(0.237)	nesosilicates & inosilicates	H
Cr_2O_3	24	151.99	(0.290)		H
			(0.247)	nesosilicates & inosilicates	H
Mn_2O_3	25	157.87	0.301		H
			0.256	nesosilicates & inosilicates	H
Fe_2O_3	26	159.69	0.315		H
			0.268	silicates	H
Co_2O_3	27	165.86	(0.329)		H
Ni_2O_3	28	165.42	(0.339)		H
Ga_2O_3	31	187.44	0.170		H
As_2O_3	33	197.84	0.235		M
Y_2O_3	39	225.81	0.170		M
			(0.195)		?
In_2O_3	49	277.64	0.130		H
Sb_2O_3	51	291.50	0.203		M
La_2O_3	57	325.82	0.148		H
Ce_2O_3	58	328.24	0.144		H
Pr_2O_3	59	329.81	0.141		H
Nd_2O_3	60	336.48	0.137		H
Pm_2O_3	61	342	(0.133)		?
Sm_2O_3	62	348.70	0.130		H
Eu_2O_3	63	351.92	0.126		H
Gd_2O_3	64	362.50	0.123		H
Tb_2O_3	65	365.85	0.119		H
Dy_2O_3	66	373.00	0.115		H
Ho_2O_3	67	377.86	0.112		H
Er_2O_3	68	382.52	0.108		H
Tm_2O_3	69	385.87	0.104		H
Yb_2O_3	70	394.08	0.101		H
Lu_2O_3	71	397.94	0.097		H
Tl_2O_3	81	456.74	0.053		M
Bi_2O_3	83	465.96	0.153		M
CO_2	6	44.01	0.211		H
SiO_2	14	60.08	0.208		H
PO_2	15	62.97	0.236		M
SO_2	16	64.06	0.262		M
TiO_2	22	79.90	0.393		H
VO_2	23	82.94	0.393		H
CrO_2	24	83.99	(0.394)		H
MnO_2	25	86.94	0.394		H
GeO_2	32	104.59	0.167		H
SeO_2	34	110.96	0.195		H
ZrO_2	40	123.22	0.211		H
SnO_2	50	150.69	0.143		H
TeO_2	52	159.60	0.201		M
CeO_2	58	172.12	(0.205)		?
HfO_2	72	210.49	0.115		M
PtO_2	78	227.09	0.151		L
PbO_2	82	239.19	0.105		M
ThO_2	90	264.04	0.167		M
UO_2	92	270.03	(0.100)		?
N_2O_5	7	108.01	0.242		H
P_2O_5	15	141.94	0.183		H
Cl_2O_5	17	150.90	0.220		H
V_2O_5	23	181.88	0.340		H
As_2O_5	33	229.84	0.162		H
Br_2O_5	35	239.81	0.180		H
Nb_2O_5	41	265.81	0.268		M
Sb_2O_5	51	323.50	(0.153)		?
I_2O_5	53	333.81	0.195		H
Ta_2O_5	73	441.89	0.151		M
Bi_2O_5	83	497.96	(0.139)		?
SO_3	16	80.06	0.177		H
CrO_3	24	99.99	0.335		M - H
SeO_3	34	126.96	0.164		H
MoO_3	42	143.94	0.237		M
TeO_3	52	175.60	0.172		M
WO_3	74	231.85	0.171		M
UO_3	92	286.03	0.118		H
S_2O_7	16	176.12	0.133		M
Cl_2O_7	17	182.90	0.182		M
Mn_2O_7	25	221.87	0.348		M
Br_2O_7	35	271.80	(0.156)		?
I_2O_7	53	365.80	0.168		M
Re_2O_7	75	484.40	0.130		L
F^-	9	19.00	0.047		M
Cl^-	17	35.45	0.318		M
Br^-	35	79.90	0.217		M
I^-	53	126.90	0.227		M
O^{2-}	8	16.00	0.203		H
S^{2-}	16	32.06	0.628	sulfur-bearing silicates	H

Constants in brackets were derived by extrapolation or interpolation. Reliability indicators: L (low), M (medium), H (high).

particular constant. For example, a constant derived from ten compounds may give a mean value with a very high standard deviation. The reliability of this constant is obviously lower than that of a constant with a low standard deviation, assuming that it has been derived from a similar number of compounds. Another factor that affects the reliability of a constant is the reliability of the constants of the other constituents in the compounds used in derivations. If constants of low reliability are used to calculate a constant, the low reliability will be passed on to the new constant.

Because of the foregoing factors, it is difficult to express the reliability of constants quantitatively. Instead, each of the constants in Table 7 is characterized by a reliability indicator expressed as L (low), M (medium) or H (high).

APPLICATION OF THE COMPATIBILITY INDEX TO SOME SETS OF MINERALOGICAL DATA

Garnet group

As stated earlier, the members of the garnet group do not yield highly compatible sets of data when the Gladstone–Dale equations are applied. However, the new constants for the trivalent constituents greatly improve the results. Because only 43 complete sets of garnet data are given by Deer *et al.* (1962a), a comparison of the compatibility using the two sets of constants for trivalent constituents would not be meaningful. Instead, data for 92 garnets were selected from *Mineralogical Abstracts* Volumes 16 to 28 (1967 to 1977). Of the 92 sets of data, all give chemical data and 88 give the index of refraction. Of the 88 sets with chemical data and the index of refraction, only 59 include measured densities. However, unit-cell edges are available for the calculation of densities in 80 cases.

Values of the compatibility index were calculated for the garnets using measured and calculated densities. For the three sets of constants used, Table 8 shows that the MR constants, as defined in the footnote to Table 8, place more garnet data in the superior category than do either of the other sets of constants.

Prior to the derivation of the new R_2O_3 constants, the garnet group seemed not to conform to the Gladstone–Dale relationship. Applying to the garnets an "end-member" approach, similar to that used by Pabst (1975) for carbonates, K_P values were computed for each of the pure end-member garnets using values of n and D(calc.) taken from the literature. These values (Table 9) were applied as k values to the weight percentages of the garnet end-members to calculate values of K_C for the previously noted garnets. These K_C values, with the K_P values calculated from n and D(calc.), were used to derive values of $1 - K_P/K_C$. The distribution among the categories of the compatibility index, in %, is: Superior 70, Excellent 25, Good 2, Fair 0 and Poor 3. This is significantly better than the corresponding data in Table 8 and indicates that, for a group like the garnets, higher compatibility is achieved if constants derived from the data for the end-members are used. However, this should be tested more fully before end-member constants are used in preference to the individual constituent constants given in Table 7. One obvious drawback to using end-member constants is the lack of good data for some end-members that may be present in significant amounts in the compound under study. For example, what end-member data would be used for garnets with high TiO_2 contents.

TABLE 8. DISTRIBUTION OF THE COMPATIBILITY INDEX AMONG CATEGORIES FOR GARNETS

	% distribution of $1-K_p/K_c$					
	using D (meas.)			using D (calc.)		
Category	L-J	M	MR	L-J	M	MR
Superior	10	19	46	0	11	51
Excellent	28	34	44	19	32	41
Good	45	40	7	51	44	4
Fair	14	7	3	20	8	0
Poor	3	0	0	10	5	4
Total	100	100	100	100	100	100
$1-K_p/K_c$ (mean)	0.046	0.038	0.020	0.053	0.046	0.023
σ	0.022	0.018	0.015	0.021	0.029	0.029
number of sets of data	58	59	59	79	80	80

L-J: K_C calculated from k-values given by Larsen (1921) and Jaffe (1956). M: k-values given by Mandarino (1976) were used.
MR: k-values given by Mandarino (1976) were used except for the trivalent constituents; for these k-values see text. Because neither Larsen nor Jaffe gave a k-value for V_2O_3, one garnet with a large amount of this constituent could not be included in the Larsen-Jaffe data.

TABLE 9. END-MEMBER CONSTANTS FOR PRINCIPAL GARNETS

End-member	K_P
pyrope	0.199
grossular	0.204
spessartine	0.191
almandine	0.192
uvarovite	0.223
andradite	0.230

Another problem lies in the quality of the data for a given end-member. The density calculated by Skinner (1956) for pyrope is 3.582 g/cm^3 and has been used in compilations of garnet data for about 25 years, but a routine check showed that the density calculated from Skinner's unit-cell edge (11.459 Å) and cell contents of 8($Mg_3Al_2Si_3O_{12}$) is 3.558 g/cm^3.

Axinite group

Lumpkin & Ribbe (1979) presented data for 39 members of the axinite group. These included indices of refraction for 12 samples, measured densities for 28 samples and calculated densities for 12 samples. In addition, they provided equations that enabled the mean index of refraction and density to be calculated from the transition metal ratio, *TM*, defined as weight percent (MnO+FeO+ZnO)/weight percent (MnO+FeO+ZnO+CaO+MgO).

These data and equations enabled K_P to be calculated in several ways. I chose the following pairs of $\bar{n}$ and *D*: (1) $\bar{n}$(obs.) and *D*(obs.), (2) $\bar{n}$(obs.) and *D*(calc. UC), (3) $\bar{n}$(calc. TM) and *D*(calc. UC), and (4) $\bar{n}$(calc. TM) and *D*(calc. TM.). *D*(calc. TM) and $\bar{n}$(calc. TM) refer to values calculated from the equations given by Lumpkin & Ribbe (1979). *D*(calc. UC) is the calculated density given by Lumpkin & Ribbe (1979), calculated by them from the unit-cell contents and parameters. K_C was calculated from the constants in Table 7 and the analyses given by Lumpkin & Ribbe. The results of the compatibility-index calculations are summarized in Table 10. Note that all the values of the compatibility index fall into the superior category. The greater superiority of the data calculated from the TM values over the other sets of data is further proof of the applicability of the equations of Lumpkin & Ribbe (1979) to the axinite group.

TABLE 10. THE COMPATIBILITY INDEX APPLIED TO THE AXINITE DATA OF LUMPKIN & RIBBE (1979)

	A	B	C	D
Number of sets of data	11	10	12	39
Range of $1-K_P/K_C$	0.000 to 0.014	0.005 to 0.019	0.005 to 0.014	0.000 to 0.010
Mean value of $1-K_P/K_C$	0.007	0.010	0.010	0.005
Standard deviation of $1-K_P/K_C$	0.005	0.005	0.002	0.002

The following data were used to calculate K_P: A, $\bar{n}$ *(obs.)* and *D (obs.)*; B, $\bar{n}$ *(obs.)* and *D (calc. UC)*; C, $\bar{n}$ *(calc. TM)* and *D (calc. UC)*; D, $\bar{n}$ *(calc. TM)* and *D (calc. TM)*. *TM* indicates values calculated from the equations given by Lumpkin & Ribbe (1979); *UC* refers to density calculated from unit cell contents and parameters.

Scapolite group

Another example of the assessment of data is provided by the chemical analyses of scapolites given by Evans *et al.* (1969) and the optical and crystallographic data of Ulbrich (1973) on the same material. Densities were calculated from the unit-cell volumes given by Ulbrich (1973) and the unit-cell contents given by Evans *et al.* (1969). The values of $1 - K_P/K_C$ are given in Table 11. The first five sets of data represent scapolites that were analyzed by "conventional" means (*i.e.*, "wet" chemical methods); the twelve other scapolites were analyzed by electron microprobe. Consequently, no values for CO_2 or H_2O were determined for the latter, and their analytical sums are significantly lower than those for which complete analyses were performed. Four of the first five sets of data fall into the superior category and one falls into the excellent category. On the other hand, none of the sets of data in the second group is characterized as superior, three are excellent, three are good and six are fair. The second and third columns show that the compatibility index of a sample is directly related to the deviation of the sample's analytical sum from 100.

New mineral descriptions

Perhaps the most important use of the compatibility index is its application to the evaluation of data for new minerals. In well-established mineral groups, it is usually possible to assess the data of a member by comparing them with the data of other group members. For new species, however, the data are often totally unrelated to those of other species. To illustrate the application to new species, calculations were

TABLE 11. COMPATIBILITY OF THE DATA OF SOME SCAPOLITES

Sample No.	$1-K_P/K_C$	Deviation of Analysis Sum from 100.00	Method of Analysis	Statistics of $1-K_P/K_C$ Values
ON8	0.005	0.25	conventional	
ON7	0.005	0.09	"	N 5
Q26	0.005	0.15	"	$\bar{X}$ 0.012
M730	0.024	0.26	"	σ 0.009
ON47	0.019	0.24	"	
M9122	0.072	6.16	probe	
17122	0.049	1.09	"	
17120	0.029	1.81	"	N 12
17139	0.033	1.98	"	$\bar{X}$ 0.054
17134	0.038	2.43	"	σ 0.014
17141	0.058	4.08	"	
17151	0.058	4.07	"	
17126	0.063	4.23	"	
17154	0.063	4.29	"	
17161	0.063	4.21	"	
17136	0.063	4.18	"	
17138	0.063	4.42	"	

Note: Sample numbers are those assigned by Evans *et al.* (1969).

carried out with the data for 34 new species published in *The Canadian Mineralogist* from 1973 through 1980. The results are given in Table 12, where they are compared with the revised data of Winchell & Winchell (1964). It appears that the data for new minerals published in *The Canadian Mineralogist* are generally of high quality.

TABLE 12. COMPATIBILITY OF DATA FROM NEW MINERAL DESCRIPTIONS

	Canadian Mineralogist		Revise Data of Winchell & Winchell (1964)
Category	Number	Percentage	Percentage
Superior	19	56	50
Excellent	9	26	22
Good	0	0	12
Fair	3	9	5
Poor	3	9	11
Total	34	100	100

CONSTANTS FOR ORGANIC CONSTITUENTS

In addition to the constants for inorganic constituents, constants for several organic constituents were calculated and are listed in Table 13. The first nine constituents are presented in oxide form and bear little resemblance to their original forms. Their constants are used in exactly the same way as most of the constants of the inorganic constituents. The last three constituents (CNS^-, CN^- and CNO^-) are presented in ion form, and their constants are used the same way as are the halide constants: an oxygen equivalent must be calculated and used in connection with the *k* value for oxygen (0.203). For a complete explanation, see Mandarino (1979, p. 74).

The constants in Table 13 were calculated from the data given by Winchell (1943). Mandarino (1976) presented a constant for oxalates (0.270), but the present constant (0.267) is considered more accurate because it was calculated from many more sets of data. The constant for formates calculated from the data given by Winchell (1943) is not considered as good as that calculated from the more accurate data given by Pabst (1978).

TABLE 13. GLADSTONE-DALE CONSTANTS FOR ORGANIC CONSTITUENTS

Name	Usual Radical Form	Oxide Form	Molecular Weight of Oxide	*k*
ethyl	$C_2H_5^+$	$(C_2H_5)_2O$	74.12	0.500
formate	HCO_2^-	$(CH)_2O_3$	74.04	0.296
				0.294*
acetate	$CH_3CO_2^-$	$(C_2H_3)_2O_3$	102.09	0.358
proprionate	$CH_3CH_2CO_2^-$	$(C_3H_5)_2O_3$	130.14	0.400
stearate	$C_{17}H_{35}CO_2^-$	$(C_{18}H_{35})_2O_3$	550.95	0.522
oxalate	$C_2O_4{}^{2-}$	C_2O_3	72.02	0.267
				0.270**
succinate	$CH_2CO_2^-$	$(C_2H_2)_2O_3$	100.07	0.340
tartrate	$C_4H_4O_6{}^{2-}$	$(CH)_4O_5$	132.07	0.305
citrate	$C_6H_5O_7{}^{3-}$	$(C_6H_5)_2O_{11}$	330.20	0.318
thiocyanate	CNS^-	———	58.08	0.461
cyanide	CN^-	———	26.02	0.391
cyanate	CNO^-	———	42.02	0.283

*from data given by Pabst (1978)

**Mandarino (1976)

CONCLUSIONS

The calculation of $1 - K_P/K_C$ provides a measure of the compatibility of the mean index of refraction, density and chemical composition. K_P should be calculated from the mean index of refraction, and the density calculated from the empirical formula. K_C is calculated from the chemical analysis using the individual *k* values.

Donnay *et al.* (1980) pointed out that the term *specific refractive energy* is a misnomer because *k* (or *K*) does not have the dimensions of an energy unit. They suggested that a better term, used by physicists, is *specific refractivity*. Their objection to the first term is quite valid. However, the second term is misleading because it implies a strong dependence on the index of refraction. In view of the uses to which I have suggested the various quantities be put, the following nomenclature is proposed. The individual *k* values for various constituents should be called the Gladstone–Dale constants. Because the *K* values calculated from the chemical composition and from the physical data are K_C and K_P, respectively, no other terms are necessary.

ACKNOWLEDGEMENTS

Many people contributed to this study, both directly and indirectly. Miss Helen Driver and Mrs. Gloria Nelson typed the manuscript and tables, respectively. Mr. Pete J. Dunn read the manuscript, made suggestions for its improvement and constantly encouraged me to finish what turned out to be a long-delayed paper. I also acknowledge the encouragement of Professor Adolf Pabst who refereed earlier parts of this series. Part IV could not have evolved without the work that constituted the first part; I thank Drs. Roland Pierrot and Claude Guillemin, who allowed me to carry out my studies at the B.R.G.M. in Orléans, France, during my tenure as a Senior Research Fellow of the National Research Council.

Studies such as this would not be possible without the assistance of those unsung heroes of science, the compilers of data; to all of them go my thanks. Finally, I thank my wife for her patience and support during countless hours of calculation.

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Received April 1981, revised manuscript accepted June 1981.