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Determination of the H_2O content in minerals, especially zeolites, from their refractive indices based on mean electronic polarizabilities of cations

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Abstract. It is shown here that the H_2O content of hydrous minerals can be determined from their mean refractive indices with high accuracy. This is especially important when only small single crystals are available. Such small crystals are generally not suitable for thermal analyses or for other reliable methods of measuring the amount of H_2O. In order to determine the contribution of the H_2O molecules to the optical properties, the total electronic polarizability is calculated from the anhydrous part of the chemical composition using the additivity rule for individual electronic polarizabilities of cations and anions. This anhydrous contribution is then compared with the total observed electronic polarizability calculated from the mean refractive index of the hydrous compound using the Anderson–Eggleton relationship. The difference between the two values represents the contribution of H_2O. The amount can be derived by solving the equation $\alpha_{\text{calc}} = \sum_i n_i \alpha_{i\text{cat}} + \sum_j \left(\alpha_j^o \times 10^{-\left[\frac{N_j}{V_\text{m}^{1.2}} \times (n_j + n_W)^{1.2}\right]} \right) + n_w \times \alpha_W$ for the number n_w of H_2O molecules per formula unit (pfu), with the electronic polarizabilities α_{cat} for cations, the values N and α^o describing the anion polarizabilities, the number n of cations and anions, and the molar volume V_m, using a value of $\alpha_W = 1.62\,\text{Å}^3$ for the electronic polarizability of H_2O. The equation is solved numerically, yielding the number n_w of H_2O molecules per formula unit. The results are compared with the observed H_2O content evaluating 157 zeolite-type compounds and 770 non-zeolitic hydrous compounds, showing good agreement. This agreement is expressed by a factor relating the calculated to the observed numbers being close to 1 for the majority of compounds. Zeolites with occluded anionic or neutral species (SO_3, SO_4, CO_2, or CO_3) show unusually high deviations between the calculated and observed amount of H_2O, indicating that the polarizabilities of these species should be treated differently in zeolites and zeolite-type compounds.

1 Introduction

The water content of hydrous minerals and synthetic compounds is usually determined by thermogravimetric methods recording the weight loss upon dehydration at an increasing temperature. If the chemical composition of the anhydrous part of the compound is known, its formula weight can be calculated along with the number of H_2O molecules representing the weight loss. Whereas the cation content can be derived from microchemical analyses, e.g., by electron microprobe analyses (EMPA) or analytical transmission electron microscopy (ATEM), on species with a size of a few microns, thermoanalytical methods for the determination of the water content require an amount of a sample in the range of a few milligrams. The same applies to carbon hydrogen and nitrogen (CHN) analyzers which usually need a few milligrams for accurate analyses. Alternatively, the H_2O content could be derived from the measured density if the specimen is big enough for the experimental determination of the density. The determination of the water content becomes less ac-

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curate if lower amounts or even just one single crystal with a size of about 100 µm and a mass of a few micrograms or less exists.

It is well known that the optical properties vary with the amount of H_2O in a crystalline compound. We mention two examples: Hey and Bannister (1932a) studied the effect of dehydration on the optical properties of natrolite, and Medenbach et al. (1980) investigated the variation in the refractive index of synthetic Mg-cordierite with H_2O content, finding a linear relationship between the mean refractive index and the weight fraction of H_2O. All studies we know so far are empirical descriptions of the dependence of the refractive indices on the H_2O content derived by calibration curves for a special system of compounds. Here, we describe a theoretical approach for determining the H_2O content from mean refractive indices of compounds with known chemical composition of the anhydrous part. We show that the number of H_2O molecules per formula unit (pfu) can be determined with high accuracy from the mean refractive indices of hydrous crystals.

A special focus is on the zeolite group of minerals, representing a large and popular group of hydrous minerals. Zeolites represent one of the most important classes of materials, used as catalysts in oil refineries for the production of gasoline and as ion exchangers as an additive, e.g., in household detergents for the softening of water. Following the definition of the subcommittee on zeolites of the International Mineralogical Association (Coombs et al., 1998), "A zeolite mineral is a crystalline substance with a structure characterized by a framework of linked tetrahedra, each consisting of four O atoms surrounding a cation. This framework contains open cavities in the form of channels and cages. These are usually occupied by H_2O molecules and extra-framework cations that are commonly exchangeable".

2 Theoretical background

Our approach is based on the fact that the total electronic polarizability of a mineral or synthetic compound can be calculated from the sum of the individual contributions of the electronic polarizabilities α_{cat} of cations and α_{an} of the anions, following the procedure described by Shannon and Fischer (2016). Thus, the total polarizability of the anhydrous compound can be calculated from the chemical composition which then can be compared with the total polarizability derived from the observed mean refractive indices of the hydrous compound. The difference represents the contribution of the H_2O molecules. To obtain the H_2O content, refractive indices are measured, e.g., by immersion methods with a spindle stage on a petrographic microscope. Anisotropic indices are averaged according to $(n_x + n_y + n_z)/3$ or $(2n_o + n_e)/3$, yielding the mean refractive index $<n>$.

The total observed polarizability of the hydrous compound is then calculated from the mean refractive index $<n>$ using the Anderson–Eggleton relationship (Anderson, 1975; Eggleton, 1991; see Shannon and Fischer, 2016, for an explanation):

$$\alpha_{\mathrm{obs}} = \frac{\left(n^2 - 1\right) V_{\mathrm{m}}}{4\pi + \left(\frac{4\pi}{3} - 2.26\right)\left(n^2 - 1\right)}, \tag{1}$$

with the molar volume V_{m} of one formula unit.

The total electronic polarizability of the anhydrous compound can be calculated from the sum of the individual ion contributions (Shannon and Fischer, 2016) according to

$$\alpha_{\mathrm{calc}} = \sum_{i=1}^{N_{\mathrm{cat}}} m_i \times \alpha_{i\mathrm{cat}} + \sum_{i=1}^{N_{\mathrm{an}}} n_i \times \alpha_{i\mathrm{an}}, \tag{2}$$

with

$$\alpha_{\mathrm{an}} = \alpha_{-}^{o} \times 10^{-N_o / V_{\mathrm{an}}^{1.2}}, \tag{3}$$

where α_{cat} is taken from Table 4 and α_{-}^{o} and N_o from Table 5 in Shannon and Fischer (2016), and the anion volume V_{an} is calculated from the molar volume V_{m} divided by the number of anions and H_2O molecules.

The difference between observed and calculated polarizabilities $\Delta = (\alpha_{\mathrm{obs}} - \alpha_{\mathrm{calc}})$ is due to the contribution of H_2O. However, Δ cannot be simply divided by the electronic polarizability 1.62 Å^3 of H_2O because it is treated like an anion and not like a cation (Shannon and Fischer, 2016). Therefore, the number n_w of H_2O molecules has an influence on the calculation of the anion volume V_{an} in Eq. (3), so it is needed to calculate the contribution of the anions even for the anhydrous part of the compound.

If we combine Eqs. (2) and (3) and separate the contribution of H_2O from the other anions, we get

$$\begin{aligned}\alpha_{\mathrm{calc}} = & \sum_i n_i \alpha_{i\mathrm{cat}} + \sum_j \left(\alpha_j^o \times 10^{-\left[\frac{N_j}{V} \times (n_j + n_W)^{1.2}\right]}\right) \\ & + n_w \times \alpha_W,\end{aligned} \tag{4}$$

with $V = V_{\mathrm{m}}^{1.2}$, the number n_w of H_2O molecules per formula unit, and the electronic polarizability $\alpha_W = 1.62$ Å^3 of H_2O.

Replacing α_{calc} in Eq. (4) by α_{obs} from Eq. (1) and solving for n_w yields the number of H_2O molecules per formula unit.

The solution is done numerically using the program POLARIO (Fischer et al., 2018).

3 Dataset

We tested the approach on hydrous minerals with known chemical composition, water content, and refractive indices, taken from Table S1 in Shannon et al. (2017) and additional entries compiled here. The group of zeolite minerals is treated separately because it represents one of the most

Table 1. Entries of zeolite-type compounds used for the comparison of observed and calculated H_2O content.

No.	Zeolite name	Chem. composition[a]	<n>[b]	V_m (Å^3)[c]	α_{obs} (Å^3)[d]	n_w (obs)[e]	n_w (calc)[f]	n_w (obs)/ n_w (calc)[g]	References[h]
1	Amicite	$K_{3.75}Na_{3.61}Ca_{0.05}Al_{7.86}Si_{8.24}O_{32} \cdot 9.67H_2O$	1.498	1052.94	87.524	9.67	13.58	0.71	Alberti et al. (1979), lp from Alberti and Vezzalini (1979)
2	Analcime synth.	$Na_{0.9}Al_{0.9}Si_{2.1}O_6 \cdot 1.1H_2O$	1.486	160.71	13.034	1.1	1.09	1.01	Černý (1974)
3	Analcime	$Na_{0.761}Cs_{0.098}K_{0.019}Ca_{0.002}Al_{0.916}Si_{2.093}O_6 \cdot 0.96H_2O$	1.492	160.50	13.179	0.96	1.02	0.94	Černý (1974)
4	Barrerite	$Na_{1.36}Ca_{0.21}Mg_{0.04}K_{0.27}Al_{2.05}Si_{6.93}O_{18} \cdot 6.45H_2O$	1.4844	553.78	44.765	6.45	6.86	0.94	Passaglia and Pongiluppi (1974)
5	Bellbergite	$Ba_{0.26}Na_{0.72}K_{1.33}Sr_{2.36}Ca_{5.32}Al_{17.55}Si_{18.36}O_{72} \cdot 30H_2O$	1.517	2429.00	209.656	30	38.59	0.78	Rüdinger et al. (1993)
6	Bikitaite	$Li_{1.05}Al_{1.00}Si_{1.99}O_6 \cdot 0.98H_2O$	1.517	147.92	12.768	0.98	0.94	1.04	Leavens et al. (1968)
7	Bikitaite	$Li_{0.915}Na_{0.005}K_{0.01}Mg_{0.015}Al_{1.10}Si_{1.95}O_6 \cdot 1.15H_2O$	1.518	148.41	12.835	1.15	1.04	1.24	Hurlbut (1957)
8	Boggsite	$Ca_{7.77}Na_{2.94}Mg_{0.13}K_{0.16}Al_{18.29}Si_{77.61}O_{192.24} \cdot 69.9H_2O$	1.483	6149.01	495.609	69.9	86.36	0.81	Howard et al. (1990)
9	Brewsterite	$Ba_{1.8}Mg_{0.08}Na_{0.07}K_{0.04}Ca_{0.03}Sr_{0.02}Al_{4.29}Fe_{0.02}Si_{11.78}O_{32} \cdot 10H_2O$	1.519	920.52	79.762	10	9.93	1.01	Cabella et al. (1993)
10	Brewsterite	$Ba_{1.7}Sr_{0.26}Ca_{0.02}K_{0.02}Na_{0.02}Al_{4.14}Si_{11.90}O_{32} \cdot 10H_2O$	1.519	919.90	79.708	10	9.95	1.01	Robinson and Grice (1993)
11	Chabazite	$Ca_{0.19}Mg_{0.19}Na_{1.64}K_{0.18}Al_{2.46}Si_{9.51}O_{24} \cdot 10.1H_2O$	1.461	807.70	62.106	10.1	10.8	0.94	Gude and Sheppard (1966)
12	Chabazite	$Na_{3.11}K_{1.05}Ca_{0.19}Mg_{0.06}Sr_{0.05}Al_{4.53}Fe_{0.01}Si_{7.40}O_{24} \cdot 11.47H_2O$	1.477	841.33	66.961	11.47	12.30	0.93	Passaglia (1970)
13	Chabazite	$Na_{2.91}K_{0.68}Ca_{0.33}Mg_{0.02}Sr_{0.03}Al_{4.15}Fe_{0.02}Si_{7.79}O_{24} \cdot 11.65H_2O$	1.479	838.10	66.986	11.65	12.65	0.92	Passaglia (1970)
14	Chabazite	$Na_{1.96}K_{0.18}Ca_{0.72}Mg_{0.01}Sr_{0.01}Al_{3.72}Fe_{0.01}Si_{8.30}O_{24} \cdot 11.97H_2O$	1.480	831.10	66.567	11.97	12.85	0.93	Passaglia (1970)
15	Chabazite	$Na_{0.17}K_{0.92}Ca_{1.30}Mg_{0.01}Sr_{0.56}Ba_{0.07}Al_{4.93}Fe_{0.01}Si_{7.05}O_{24} \cdot 13.20H_2O$	1.516	844.62	72.761	13.20	15.13	0.87	Passaglia (1970)
16	Chabazite	$Na_{0.28}K_{1.36}Ca_{1.04}Mg_{0.02}Sr_{0.40}Ba_{0.06}Al_{4.87}Fe_{0.01}Si_{7.17}O_{24} \cdot 13.16H_2O$	1.517	850.28	73.391	13.16	15.61	0.84	Passaglia (1970)
17	Chabazite	$Na_{0.09}K_{0.86}Ca_{1.38}Mg_{0.02}Sr_{0.48}Ba_{0.09}Al_{4.84}Fe_{0.02}Si_{7.14}O_{24} \cdot 13.91H_2O$	1.514	846.93	72.675	13.91	15.10	0.92	Passaglia (1970)
18	Chabazite	$Na_{0.15}K_{1.08}Ca_{1.31}Mg_{0.03}Sr_{0.57}Ba_{0.04}Al_{4.92}Fe_{0.02}Si_{7.02}O_{24} \cdot 13.55H_2O$	1.516	845.35	72.823	13.55	15.04	0.90	Passaglia (1970)
19	Chabazite	$Na_{0.31}K_{0.41}Ca_{1.30}Mg_{0.10}Sr_{0.04}Ba_{0.01}Al_{3.59}Fe_{0.17}Si_{8.28}O_{24} \cdot 12.49H_2O$	1.498	828.00	68.826	12.49	13.60	0.92	Passaglia (1970)
20	Chabazite	$Na_{1.59}K_{0.13}Ca_{1.13}Mg_{0.01}Sr_{0.01}Al_{3.93}Fe_{0.01}Si_{8.04}O_{24} \cdot 14.22H_2O$	1.486	829.74	67.296	14.22	13.07	1.09	Passaglia (1970)
21	Chabazite	$Na_{0.27}K_{0.21}Ca_{1.39}Mg_{0.02}Sr_{0.05}Al_{3.38}Fe_{0.02}Si_{8.60}O_{24} \cdot 12.95H_2O$	1.486	825.04	66.915	12.95	12.89	1.00	Passaglia (1970)
22	Chabazite	$Na_{0.11}K_{0.04}Ca_{1.45}Mg_{0.01}Sr_{0.61}Al_{4.17}Fe_{0.01}Si_{7.80}O_{24} \cdot 14.61H_2O$	1.506	831.32	70.219	14.61	14.34	1.02	Passaglia (1970)
23	Chabazite	$Na_{0.06}K_{0.48}Ca_{1.31}Mg_{0.02}Sr_{0.15}Al_{3.60}Fe_{0.02}Si_{8.41}O_{24} \cdot 12.66H_2O$	1.492	827.08	67.915	12.66	13.28	0.95	Passaglia (1970)
24	Chabazite	$Na_{0.03}K_{0.20}Ca_{1.86}Mg_{0.02}Sr_{0.03}Al_{3.94}Fe_{0.01}Si_{8.03}O_{24} \cdot 13.16H_2O$	1.498	825.63	68.629	13.16	13.57	0.97	Passaglia (1970)
25	Chabazite	$Na_{0.09}K_{0.18}Ca_{1.55}Mg_{0.06}Sr_{0.13}Al_{3.73}Fe_{0.01}Si_{8.26}O_{24} \cdot 12.84H_2O$	1.494	825.09	68.029	12.84	13.38	0.96	Passaglia (1970)
26	Chabazite	$Na_{0.16}K_{0.40}Ca_{1.03}Mg_{0.15}Sr_{0.06}Ba_{0.03}Al_{3.23}Si_{8.80}O_{24} \cdot 15.25H_2O$	1.488	826.68	67.326	15.25	13.31	1.15	Passaglia (1970)
27	Chabazite	$Na_{1.45}K_{0.38}Ca_{1.03}Mg_{0.01}Sr_{0.07}Ba_{0.02}Al_{4.10}Fe_{0.01}Si_{7.90}O_{24} \cdot 12.57H_2O$	1.490	835.61	68.334	12.57	13.48	0.93	Passaglia (1970)
28	Chabazite	$Na_{0.92}K_{0.13}Ca_{1.25}Mg_{0.01}Sr_{0.04}Ba_{0.01}Al_{3.77}Si_{8.25}O_{24} \cdot 12.85H_2O$	1.488	828.48	67.473	12.85	13.21	0.97	Passaglia (1970)
29	Chabazite	$Na_{1.28}K_{0.52}Ca_{1.00}Mg_{0.01}Sr_{0.05}Al_{3.85}Fe_{0.01}Si_{8.14}O_{24} \cdot 13.11H_2O$	1.488	832.52	67.802	13.11	13.21	0.99	Passaglia (1970)
30	Chabazite[i]	$Na_{0.17}K_{0.15}Ca_{1.70}Mg_{0.01}Sr_{0.01}Al_{3.72}Si_{8.27}O_{24} \cdot 13.92H_2O$	1.496	825.72	68.359	13.92	13.65	1.02	Passaglia (1970)
31	Chabazite	$Na_{0.44}K_{0.15}Ca_{1.65}Mg_{0.03}Al_{3.80}Si_{8.16}O_{24} \cdot 12.47H_2O$	1.496	833.22	68.980	12.47	14.00	0.89	Passaglia (1970)
32	Chabazite	$Na_{0.35}K_{0.10}Ca_{1.48}Sr_{0.04}Ba_{0.08}Al_{3.53}Si_{8.44}O_{24} \cdot 12.66H_2O$	1.495	818.91	67.657	12.66	13.26	0.95	Passaglia (1970)
33	Chabazite	$Na_{0.19}K_{0.23}Ca_{1.15}Sr_{0.20}Ba_{0.14}Al_{3.44}Si_{8.58}O_{24} \cdot 12.24H_2O$	1.492	822.46	67.536	12.24	13.11	0.93	Passaglia (1970)
34	Chabazite	$Na_{0.17}K_{0.32}Ca_{1.49}Mg_{0.02}Sr_{0.04}Ba_{0.04}Al_{3.39}Si_{8.55}O_{24} \cdot 12.44H_2O$	1.495	824.84	68.147	12.44	13.52	0.92	Passaglia (1970)
35	Chabazite	$Na_{0.03}K_{0.42}Ca_{0.99}Sr_{0.41}Ba_{0.05}Al_{3.67}Si_{8.41}O_{24} \cdot 12.77H_2O$	1.487	826.28	67.154	12.77	12.75	1.00	Passaglia (1970)
36	Chabazite	$Na_{1.64}K_{0.13}Ca_{0.19}Mg_{0.19}Al_{2.46}Fe_{0.02}Si_{9.51}O_{24} \cdot 10.10H_2O$	1.461	806.27	61.996	10.10	10.70	0.94	Passaglia (1970)
37	Chiavennite	$Ca_{0.92}Na_{0.12}Mn_{0.80}Fe_{0.15}Mg_{0.02}Be_{1.86}Al_{0.14}Al_{0.57}Si_{4.43}O_{12.45}(OH)_{2.49}F_{0.06} \cdot 1.83H_2O$	1.6047	332.55	33.567	1.83	2.55	0.72	Raade et al. (1983)
38	Clinoptilolite	$Na_{2.10}Ca_{0.48}K_{1.64}Mg_{0.23}Al_{0.24}Al_{5.83}Si_{30.17}O_{72} \cdot 24.0H_2O$	1.479	2100.3	167.869	24.0	21.65	1.11	Wise et al. (1969)
39	Dachiardite	$Na_{2.93}K_{0.36}Sr_{0.01}Al_{3.59}Si_{20.47}O_{48} \cdot 12.76H_2O$	1.474	1361.2	107.649	12.76	12.47	1.02	Bonardi et al. (1981)
40	Dachiardite	$Ca_{0.53}Mg_{0.04}Ba_{0.01}Na_{2.59}K_{0.71}Al_{4.27}Fe_{0.11}Si_{19.61}O_{48} \cdot 13.43H_2O$Bao.26Nao.72K1.33Sr2.36Ca5.32Al	1.481	1367.64	109.771	13.43	12.59	1.07	Alberti (1975)
41	Direnzoite	$Na_{1.12}K_{2.73}Mg_{1.56}Ca_{2.17}Fe_{0.15}Sr_{0.03}Ba_{0.01}Al_{13.40}Si_{46.98}O_{120} \cdot 35.99H_2O$	1.483	3607.74	290.783	35.99	40.27	0.89	Galli and Gualtieri (2008)
42	Edingtonite	$Ba_{0.96}K_{0.035}Al_{2.085}Si_{3.115}O_{10.33} \cdot 3.67H_2O$	1.541	300.98	27.189	3.67	3.26	1.13	Grice et al. (1984)
43	Edingtonite	$Ba_{1.00}K_{0.01}Al_{2.115}Si_{3.10}O_{10.39} \cdot 3.61H_2O$	1.546	300.47	27.394	3.61	3.26	1.11	Grice et al. (1984)
44	Edingtonite	$Ba_{1.015}Ca_{0.01}Na_{0.01}K_{0.07}Al_{1.985}Si_{2.98}O_{10.04} \cdot 3.69H_2O$	1.550	302.14	27.748	3.69	3.82	0.97	Hey and Bannister (1934)

Table 1. Continued

No.	Zeolite name	Chem. composition[a]	<n>[b]	V_m (Å^3)[c]	α_obs (Å^3)[d]	n_w (obs)[e]	n_w (calc)[f]	n_w (obs)/ n_w (calc)[g]	References[h]
45	Edingtonite	$\mathrm{Ba_{0.835}Al_{2.145}Si_{2.97}O_{10.40} \cdot 3.34H_2O}$	1.545	299.97	27.398	3.34	3.58	0.93	Hey and Bannister (1934)
46	Erionite	$\mathrm{Mg_{0.86}Ca_{2.26}Na_{0.96}K_{1.54}Al_{8.80}Fe_{0.38}Si_{26.82}O_{71.78} \cdot 31.2H_2O}$	1.478	2295.5	183.084	31.2	28.2	1.11	Sheppard and Gude (1969)
47	Erionite	$\mathrm{Mg_{0.78}Ca_{1.48}Na_{1.34}K_{2.06}Al_{8.74}Si_{27.26}O_{71.60} \cdot 27.8H_2O}$	1.469	2297.4	179.752	27.8	27.3	1.02	Sheppard and Gude (1969)
48	Erionite	$\mathrm{Mg_{0.10}Fe_{0.08}Na_{5.80}K_{2.50}Ti_{0.12}Mn_{0.12}Al_{7.86}Fe_{0.70}Si_{27.42}P_{0.02}O_{72.40} \cdot 24.4H_2O}$	1.465	2281.9	177.000	24.4	22.6	1.08	Sheppard and Gude (1969)
49	Erionite	$\mathrm{Mg_{0.48}Fe_{0.04}Ca_{0.48}Na_{2.76}K_{2.90}Ti_{0.06}Al_{7.58}Fe_{0.76}Si_{27.66}O_{71.78}F_{0.02} \cdot 23.6H_2O}$	1.465	2282.1	177.016	23.6	23.5	1.00	Sheppard and Gude (1969)
50	Erionite	$\mathrm{Mg_{0.10}Na_{5.38}K_{2.18}Ti_{0.02}Al_{7.84}Fe_{0.26}Si_{27.90}O_{71.88}F_{0.02} \cdot 23.8H_2O}$	1.459	2276.6	174.286	23.8	23.4	1.02	Sheppard and Gude (1969)
51	Erionite	$\mathrm{Mg_{0.82}Ca_{1.36}Na_{0.58}K_{2.94}Ti_{0.04}Al_{7.94}Fe_{0.14}Si_{27.90}P_{0.02}O_{71.98}Cl_{0.02}F_{0.02} \cdot 26.2H_2O}$	1.468	2278.6	177.897	26.2	25.1	1.04	Sheppard and Gude (1969)
52	Erionite	$\mathrm{Mg_{0.18}Fe_{0.02}Ca_{0.10}Na_{5.52}K_{1.98}Ti_{0.06}Mn_{0.02}Al_{7.48}Fe_{0.52}Si_{27.98}P_{0.02}O_{72.18} \cdot 24.4H_2O}$	1.464	2275.5	176.120	24.4	24.6	0.99	Sheppard and Gude (1969)
53	Erionite	$\mathrm{Mg_{0.34}Ca_{0.66}Na_{3.16}K_{2.58}Ti_{0.04}Al_{7.34}Fe_{0.46}Si_{28.20}O_{72.02}Cl_{0.02}F_{0.08} \cdot 23.6H_2O}$	1.465	2274.0	176.388	23.6	23.7	1.00	Sheppard and Gude (1969)
54	Erionite	$\mathrm{Mg_{0.76}Fe_{0.04}Ca_{0.32}Na_{3.98}K_{2.44}Ti_{0.04}Mn_{0.02}Al_{7.12}Fe_{0.48}Si_{28.40}O_{72.62} \cdot 22.8H_2O}$	1.462	2274.4	175.268	22.8	22.4	1.02	Sheppard and Gude (1969)
55	Erionite	$\mathrm{Na_{1.01}K_{2.84}Mg_{0.3}Ca_{1.69}Al_{8.18}Si_{27.84}O_{72} \cdot 28.51H_2O}$	1.469	2267.1	177.381	28.51	25.0	1.14	Gude and Sheppard (1981)
56	Erionite	$\mathrm{K_{1.56}Na_{0.96}Mg_{0.84}Ca_{2.28}Al_{8.94}Si_{27.30}O_{72} \cdot 31.20H_2O}$	1.479	2295.4	183.463	31.20	29.1	1.07	Harada et al. (1967)
57	Erionite	$\mathrm{Ca_{1.76}Mg_{0.48}K_{2.21}Na_{2.26}Al_{8.95}Si_{27.00}O_{71.9} \cdot 27.2H_2O}$	1.473	2274.01	179.455	27.2	26.3	1.03	Deffeyes (1959)
58	Erionite	$\mathrm{Ca_{1.61}Mg_{0.61}K_{2.06}Na_{1.77}Al_{8.70}Si_{26.74}O_{70.65} \cdot 27.2H_2O}$	1.470	2302.34	180.527	27.2	28.7	0.95	Staples and Gard (1959)
59	Faujasite-Ca	$\mathrm{Ca_{0.95}Mg_{0.22}Na_{1.04}K_{0.02}Al_{3.4}Si_{8.6}O_{24} \cdot 16H_2O}$	1.466	934.75	72.663	16	16.8	0.95	Wise (1982)
60	Ferrierite	$\mathrm{K_{0.51}Na_{0.25}Ca_{0.99}Mg_{2.98}Al_{7.25}Fe_{1.20}Si_{27.50}O_{72} \cdot 23.12H_2O}$	1.490	2085.9	170.580	23.12	20.3	1.14	Alietti and Passagli (1967)
61	Ferrierite-K	$\mathrm{Na_{1.32}K_{1.57}Mg_{1.09}Al_{5.03}Fe_{0.01}Si_{30.95}O_{72.01} \cdot 18.82H_2O}$	1.484	2032.84	164.189	18.82	20.1	0.94	Yajima and Nakamura (1971) lp from Alietti and Passaglia (1967)
62	Ferrierite-$\mathrm{NH_4}$	$\mathrm{H_{0.35}(NH_4)_{2.74}Mg_{1.07}Na_{0.21}Al_{5.44}Si_{30.56}O_{72} \cdot 21.55H_2O}$.	1.520	2024.0	175.717	21.55	25.8	0.84	Chukanov et al. (2019)
63	Ferrochiavennite	$\mathrm{Ca_{1.73}Na_{0.13}Fe_{0.41}Mn_{0.31}Mg_{0.02}Si_{4.22}Al_{0.50}Be_{2.28}O_{13}(OH)_2 \cdot 2H_2O}$	1.591	332.92	32.848	2	1.7	1.18	Grice et al. (2013)
64	Flörkeite	$\mathrm{K_{2.96}Ca_{2.04}Na_{1.02}Mg_{0.01}Al_{8.03}Si_{7.97}O_{31.97} \cdot 11.72H_2O}$	1.513	1014.1	86.850	11.72	12.7	0.92	Lengauer et al. (2009)
65	Gaultite	$\mathrm{Na_{4.28}Zn_{1.88}Si_{6.99}O_{18} \cdot 5H_2O}$	1.522	524.5	45.711	5	5.5	0.91	Ercit and van Velthuizen (1994)
66	Gismondine	$\mathrm{Ca_{0.905}K_{0.06}Na_{0.025}Sr_{0.005}Al_{1.87}Si_{2.115}O_8 \cdot 4.5H_2O}$	1.538	261.3	23.473	4.5	4.7	0.96	Vezzalini and Oberti (1984)
67	Gobbinsite	$\mathrm{Mg_{0.31}Sr_{0.04}Ca_{0.35}Ba_{0.01}Na_{3.98}K_{0.18}Al_{5.80}Fe_{0.01}Si_{10.25}O_{32} \cdot 12H_2O}$	1.492	1007.4	82.722	12	13.4	0.90	Nawaz and Malone (1982)
68	Goosecreekite	$\mathrm{Ca_{2.02}Al_{4.10}Si_{12.00}O_{32.17} \cdot 10.12H_2O}$	1.498	934.3	77.662	10.12	10.3	0.98	Dunn et al. (1980)
69	Gottardiite	$\mathrm{Na_{2.5}K_{0.20}Mg_{3.10}Ca_{4.8}Al_{18.80}Si_{117.2}O_{272} \cdot 93H_2O}$	1.484	7826.0	632.092	93	84.7	1.10	Galli et al. (1996)
70	Harmotome	$\mathrm{Mg_{0.17}Ca_{0.02}Ba_{1.98}Na_{0.86}K_{0.07}Al_{4.39}Fe_{0.14}Si_{11.05}O_{31.53} \cdot 12.69H_2O}$	1.508	999.2	84.735	12.69	12.6	1.01	Sahama and Lehtinen (1967)
71	Heulandite	$\mathrm{Ca_{3.5}Sr_{0.4}K_{0.9}Al_{9.3}Si_{26.8}O_{72} \cdot 26.1H_2O}$	1.499	2104.0	175.241	26.1	23.7	1.10	Merkle and Slaughter (1968)
72	Heulandite-Ba	$\mathrm{Ba_{2.49}Ca_{1.41}Sr_{0.30}K_{0.37}Na_{0.33}Al_{8.96}Si_{27.00}O_{72.00} \cdot 21.75H_2O}$	1.509	2102.0	178.609	21.75	23.4	0.93	Larsen et al. (2005)
73	Heulandite-Sr	$\mathrm{Na_{1.44}K_{0.83}Ca_{1.57}Sr_{1.25}Ba_{0.46}Mg_{0.06}Al_{9.05}Si_{26.97}O_{72} \cdot 25H_2O}$	1.509	2181.4	185.352	25	30.2	0.83	Černý and Povondra (1969)
74	Laumontite	$\mathrm{Ca_{3.35}Na_{0.77}K_{0.27}Al_{8.24}Si_{15.87}O_{48} \cdot 17.10H_2O}$	1.515	1361.8	117.085	17.10	15.1	1.13	Tomita et al. (1979)
75	Leonhardite	$\mathrm{Ca_{2.55}Na_{1.24}K_{1.59}Al_{8.19}Si_{15.87}O_{48} \cdot 13.93H_2O}$	1.509	1352.7	114.940	13.93	13.2	1.06	Kiseleva et al. (1996b)
76	Leonhardite	$\mathrm{Ca_{4.02}Na_{0.03}K_{0.05}Mn_{0.02}Mg_{0.02}Al_{7.98}Si_{15.96}P_{0.03}O_{48} \cdot 14.07H_2O}$	1.513	1346.7	115.332	14.07	13.7	1.03	Kiseleva et al. (1996a) RI from Kiseleva et al. (1996b)
77	Levyne	$\mathrm{Ca_{2.50}Na_{0.84}K_{0.06}Al_{6.11}Si_{11.94}O_{36} \cdot 16.98H_2O}$	1.498	1173.9	97.598	16.98	17.4	0.98	Passaglia et al. (1974)
78	Levyne	$\mathrm{Ca_{2.36}Na_{0.82}K_{0.33}Al_{5.58}Si_{12.35}O_{36} \cdot 16.14H_2O}$	1.488	1178.6	95.987	16.14	16.3	0.99	Passaglia et al. (1974)
79	Levyne	$\mathrm{Ca_{2.73}Na_{0.65}K_{0.20}Al_{6.31}Si_{11.69}O_{36} \cdot 16.66H_2O}$	1.507	1181.9	100.030	16.66	18.6	0.90	Passaglia et al. (1974)
80	Levyne	$\mathrm{Na_{0.96}K_{0.24}Ca_{2.88}Al_{6.81}Si_{11.16}O_{36} \cdot 17.4H_2O}$	1.496	1181.4	97.804	17.4	16.8	1.04	Tiba and Matsubara (1977)
81	Lovdarite	$\mathrm{Na_{12.32}K_{3.40}Ca_{2.24}Ba_{0.04}Be_{7.04}Al_{0.80}Ti_{0.04}Fe_{0.04}Mg_{0.04}Si_{23.88}Al_{0.08}P_{0.04}O_{64.56} \cdot 17.48H_2O}$	1.516	1843.0	158.767	17.48	19.19	0.91	Men’shikov et al. (1973)
82	Mazzite	$\mathrm{Na_{0.03}K_{1.91}Ca_{1.35}Mg_{1.99}Al_{9.77}Si_{26.54}O_{72} \cdot 28.03H_2O}$	1.504	2239.9	188.446	28.03	33.0	0.85	Galli et al. (1974)
83	Merlinoite	$\mathrm{K_{4.21}Ca_{1.49}Na_{0.55}Ba_{0.24}Fe_{0.24}Al_{9.31}Si_{22.66}O_{64} \cdot 22.74H_2O}$	1.494	1997.7	164.712	22.74	24.24	0.94	Passaglia et al. (1977)
84	Montesommaite	$\mathrm{K_{8.6}Na_{0.2}Al_{9.4}Si_{22.6}O_{63.7} \cdot 10.25H_2O}$	1.504	1765.1	148.500	10.25	13.5	0.76	Rouse et al. (1990)
85	Mordenite-Sr	$\mathrm{Ca_{2.02}Sr_{0.46}Na_{3.12}K_{0.36}Al_{8.32}Si_{39.66}O_{96} \cdot 30.1H_2O}$	1.483	2785.2	224.487	30.1	34.6	0.87	Reay and Coombs (1971)
86	Nabesite	$\mathrm{Na_{1.74}K_{0.03}Ca_{0.01}Be_{0.98}Si_{4.06}O_{10} \cdot 3.92H_2O}$	1.506	295.2	24.934	3.92	4.08	0.96	Petersen et al. (2002)

Table 1. Continued

No.	Zeolite name	Chem. composition[a]	$\langle n \rangle$[b]	V_m (Å^3)[c]	α_{obs} (Å^3)[d]	n_w (obs)[e]	n_w (calc)[f]	n_w (obs)/ n_w (calc)[g]	References[h]
87	Natrolite	$Na_{1.80}K_{0.04}Ca_{0.02}Al_{2.05}Si_{2.98}O_{10} \cdot 2H_2O$	1.484	281.0	22.697	2	2.2	0.91	
88	Natrolite	$Ca_{0.18}Na_{1.75}Al_{2.03}Si_{2.95}O_{10} \cdot 2.10H_2O$	1.482	280.7	22.575	2.10	1.97	1.07	Cortesogno et al. (1975)
89	Natrolite	$Ca_{0.04}K_{0.03}Na_{1.82}Al_{2.05}Si_{2.98}O_{10} \cdot 2.01H_2O$	1.484	281.9	22.769	2.01	2.19	0.92	Hey and Bannister (1932a)
90	Natrolite	$Ca_{0.007}Na_{2.014}K_{0.004}Ti_{0.002}Fe_{0.002}Al_{1.916}Si_{3.084}O_{10.065} \cdot 2.09H_2O$	1.483	280.95	22.645	2.09	2.06	1.01	Chen and Chao (1980)
91	Offretite	$Mg_{0.72}Ca_{1.06}Na_{0.47}K_{1.11}Al_{5.17}Si_{12.83}O_{36} \cdot 15.2H_2O$	1.488	1159.9	94.464	15.2	15.9	0.96	Sheppard and Gude (1969)
92	Pahasapaite	$Ca_{5.5}Li_{11.6}K_{1.2}Na_{0.2}Be_{24}P_{24}O_{96} \cdot 38H_2O$	1.523	2617.2	228.533	38	34.5	1.10	Rouse et al. (1987)
93	Parthéite	$Ca_{2.00}Na_{0.06}Al_{4.20}Si_{4.40}O_{16} \cdot 4H_2O$	1.552	441.0	40.648	4	5.0	0.80	Sarp et al. (1979)
94	Paulingite	$Ca_{2.57}Ba_{1.39}K_{2.28}Na_{0.38}Al_{11.55}Si_{30.59}O_{84} \cdot 27H_2O$	1.482	2708.06	217.813	27	33.5	0.81	Lengauer et al. (1997)
95	Perlialite	$K_{9.07}Na_{0.91}Ca_{0.49}Sr_{0.46}Fe_{0.08}Al_{11.35}Fe_{0.33}Mg_{0.05}Si_{24.27}O_{72.12} \cdot 15.2H_2O$	1.485	2223.5	179.962	15.2	20.5	0.74	Men'chikov (1984)
96	Phillipsite	$K_{1.58}Na_{1.36}Ca_{1.36}Al_{5.62}Fe_{0.16}Si_{10.24}O_{32} \cdot 12.78H_2O$	1.485	1008.41	81.617	12.78	11.1	1.15	Harada et al. (1967)
97	Phillipsite	$Mg_{0.01}Ca_{1.79}Sr_{0.03}Na_{0.63}K_{2.28}Al_{6.37}Fe_{0.02}Si_{9.57}O_{32} \cdot 12.87H_2O$	1.506	1020.85	86.228	12.87	13.4	0.96	Galli and Loschi Ghittoni (1972)
98	Phillipsite	$Mg_{0.02}Ca_{0.66}Sr_{0.01}Ba_{0.01}Na_{1.05}K_{3.56}Al_{6.18}Fe_{0.01}Si_{9.86}O_{32} \cdot 11.51H_2O$	1.494	1024.8	84.495	11.51	12.2	0.94	Galli and Loschi Ghittoni (1972)
99	Phillipsite	$Mg_{0.01}Ca_{2.09}Sr_{0.04}Ba_{0.01}Na_{0.29}K_{1.99}Al_{6.45}Fe_{0.01}Si_{9.51}O_{32} \cdot 13.54H_2O$	1.504	1014.4	85.339	13.54	12.9	1.05	Galli and Loschi Ghittoni (1972)
100	Phillipsite	$Mg_{0.01}Ca_{1.97}Sr_{0.03}Ba_{0.01}Na_{0.42}K_{2.40}Al_{6.37}Fe_{0.01}Si_{9.51}O_{32} \cdot 13.09H_2O$	1.504	1020.15	85.827	13.09	13.0	1.01	Galli and Loschi Ghittoni (1972)
101	Phillipsite	$Mg_{0.01}Ca_{2.02}Sr_{0.04}Ba_{0.03}Na_{0.45}K_{1.91}Al_{6.83}Fe_{0.02}Si_{9.22}O_{32} \cdot 13.91H_2O$	1.504	1014.9	85.385	13.91	12.9	1.08	Galli and Loschi Ghittoni (1972)
102	Phillipsite	$Mg_{0.03}Ca_{0.26}Sr_{0.01}Ba_{0.01}Na_{4.18}K_{0.68}Al_{5.64}Fe_{0.01}Si_{10.41}O_{32} \cdot 13.67H_2O$	1.494	1017.6	83.898	13.67	13.9	0.98	Galli and Loschi Ghittoni (1972)
103	Phillipsite	$Mg_{0.02}Ca_{0.64}Sr_{0.01}Ba_{0.03}Na_{3.35}K_{0.93}Al_{5.66}Fe_{0.01}Si_{10.33}O_{32} \cdot 12.41H_2O$	1.498	1017.6	84.586	12.41	14.0	0.89	Galli and Loschi Ghittoni (1972)
104	Phillipsite	$Mg_{0.01}Ca_{0.41}Ba_{0.01}Na_{4.19}K_{0.89}Al_{5.66}Fe_{0.01}Si_{10.27}O_{32} \cdot 12.25H_2O$	1.498	1018.7	84.673	12.25	14.2	0.86	Galli and Loschi Ghittoni (1972)
105	Phillipsite	$Mg_{0.01}Ca_{1.34}Sr_{0.01}Ba_{0.05}Na_{1.00}K_{1.87}Al_{5.79}Fe_{0.01}Si_{10.24}O_{32} \cdot 12.06H_2O$	1.499	1013.5	84.416	12.06	13.0	0.93	Galli and Loschi Ghittoni (1972)
106	Phillipsite	$Mg_{0.01}Ca_{0.54}Ba_{0.02}Na_{3.56}K_{0.93}Al_{5.38}Fe_{0.01}Si_{10.55}O_{32} \cdot 12.82H_2O$	1.496	1017.3	84.215	12.82	13.9	0.92	Galli and Loschi Ghittoni (1972)
107	Phillipsite	$Mg_{0.02}Ca_{0.51}Ba_{0.01}Na_{1.40}K_{3.79}Al_{6.56}Fe_{0.01}Si_{9.50}O_{32} \cdot 13.49H_2O$	1.502	1025.8	85.957	13.49	13.0	1.04	Galli and Loschi Ghittoni (1972)
108	Phillipsite	$Mg_{0.03}Ca_{1.48}Sr_{0.01}Ba_{0.10}Na_{0.21}K_{0.68}Al_{4.13}Fe_{0.03}Si_{11.85}O_{32} \cdot 12.85H_2O$	1.500	1007.4	84.073	12.85	14.1	0.91	Galli and Loschi Ghittoni (1972)
109	Phillipsite	$Mg_{0.04}Ca_{1.46}Sr_{0.02}Ba_{0.10}Na_{0.43}K_{1.13}Al_{4.87}Fe_{0.04}Si_{11.13}O_{32} \cdot 13.41H_2O$	1.500	1015.9	84.782	13.41	13.9	0.96	Galli and Loschi Ghittoni (1972)
110	Phillipsite	$Mg_{0.07}Ca_{1.16}Sr_{0.01}Ba_{0.05}Na_{0.18}K_{1.85}Al_{4.58}Fe_{0.02}Si_{11.40}O_{32} \cdot 12.30H_2O$	1.490	1010.5	82.637	12.30	12.5	0.98	Galli and Loschi Ghittoni (1972)
111	Phillipsite	$Mg_{0.03}Ca_{1.82}Sr_{0.01}Ba_{0.03}Na_{0.08}K_{1.83}Al_{5.63}Fe_{0.02}Si_{10.34}O_{32} \cdot 12.87H_2O$	1.502	1010.4	84.667	12.87	13.1	0.98	Galli and Loschi Ghittoni (1972)
112	Phillipsite	$Mg_{0.01}Ca_{2.12}Na_{0.20}K_{1.80}Al_{6.19}Fe_{0.04}Si_{9.76}O_{32} \cdot 12.93H_2O$	1.508	1012.3	85.842	12.93	13.4	0.96	Galli and Loschi Ghittoni (1972)
113	Phillipsite	$Mg_{0.01}Ca_{1.25}Sr_{0.01}Na_{0.57}K_{1.71}Al_{5.04}Fe_{0.01}Si_{11.01}O_{32} \cdot 12.67H_2O$	1.503	1014.1	85.147	12.67	14.1	0.90	Galli and Loschi Ghittoni (1972)
114	Phillipsite	$Mg_{0.01}Ca_{1.75}Sr_{0.01}Ba_{0.06}Na_{0.17}K_{1.86}Al_{5.74}Fe_{0.01}Si_{10.27}O_{32} \cdot 12.57H_2O$	1.507	1010.2	85.494	12.57	13.6	0.92	Galli and Loschi Ghittoni (1972)
115	Phillipsite	$Mg_{0.01}Ca_{1.77}Na_{0.16}K_{1.87}Al_{5.77}Fe_{0.01}Si_{10.27}O_{32} \cdot 12.28H_2O$	1.503	1010.8	84.866	12.28	13.3	0.92	Galli and Loschi Ghittoni (1972)
116	Phillipsite	$Mg_{0.01}Ca_{1.84}Sr_{0.01}Ba_{0.08}Na_{0.16}K_{1.94}Al_{5.75}Fe_{0.01}Si_{10.19}O_{32} \cdot 12.27H_2O$	1.509	1007.7	85.625	12.27	13.5	0.91	Galli and Loschi Ghittoni (1972)
117	Phillipsite	$Mg_{0.01}Ca_{0.91}Na_{0.74}K_{1.83}Al_{5.65}Si_{10.41}O_{32} \cdot 12.25H_2O$	1.498	1015.6	84.416	12.25	13.8	0.89	Galli and Loschi Ghittoni (1972)
118	Phillipsite	$Mg_{0.01}Ca_{2.01}Na_{0.09}K_{1.55}Al_{6.69}Fe_{0.02}Si_{9.30}O_{32} \cdot 13.78H_2O$	1.508	1013.85	85.978	13.78	13.9	0.99	Galli and Loschi Ghittoni (1972)
119	Phillipsite	$Mg_{0.01}Ca_{1.60}Na_{0.13}Ba_{0.38}K_{0.71}Al_{5.00}Fe_{0.03}Si_{11.02}O_{32} \cdot 12.97H_2O$	1.502	1011.3	84.738	12.97	13.7	0.95	Galli and Loschi Ghittoni (1972)
120	Pollucite	$Na_{0.357}Cs_{0.445}K_{0.009}Li_{0.015}Ca_{0.004}Al_{0.861}Si_{2.127}O_6 \cdot 0.54H_2O$	1.507	158.61	13.424	0.54	0.60	0.90	Černý (1974)
121	Pollucite	$Na_{0.181}Cs_{0.551}Rb_{0.017}K_{0.103}Li_{0.028}Ca_{0.001}Al_{0.937}Si_{2.061}O_6 \cdot 0.41H_2O$	1.520	159.80	13.873	0.41	0.61	0.67	Černý (1974)
122	Pollucite	$Na_{0.182}Cs_{0.658}K_{0.036}Al_{0.924}Si_{2.088}O_6 \cdot 0.31H_2O$	1.520	158.96	13.800	0.31	0.43	0.72	Černý (1974)
123	Pollucite	$Na_{0.163}Cs_{0.747}Rb_{0.031}K_{0.004}Li_{0.010}Al_{0.851}Si_{2.140}O_6 \cdot 0.23H_2O$	1.520	159.31	13.831	0.23	0.26	0.88	Černý (1974)
124	Pollucite	$Na_{0.143}Cs_{0.628}Rb_{0.021}Li_{0.002}Mn_{0.001}Al_{0.944}Si_{2.071}O_6 \cdot 0.29H_2O$	1.517	160.29	13.835	0.29	0.52	0.56	Černý (1974)
125	Pollucite	$Na_{0.146}Cs_{0.722}K_{0.023}Ca_{0.001}Al_{0.909}Si_{2.092}O_6 \cdot 0.25H_2O$	1.520	158.96	13.800	0.25	0.32	0.78	Černý (1974)
126	Pollucite	$Cs_{0.097}Ca_{0.002}Na_{0.760}K_{0.019}Al_{0.913}Si_{2.087}O_{5.984} \cdot 1.00H_2O$	1.492	160.50	13.179	1.00	1.03	0.97	Černý (1972)
127	Roggianite	$Ca_{14.24}Sr_{0.01}Na_{0.37}K_{0.56}Be_{5.29}Al_{14.92}Si_{27.79}O_{89.96}(OH)_{16} \cdot 1H_2O$	1.530	3100.2	274.345	33.68	38.7	0.87	Passaglia and Vezzalini (1988) RI from Passaglia (1969)
128	Scolecite	$Ca_{1.045}Na_{0.020}K_{0.004}Al_{2.005}Si_{2.966}O_{10.025} \cdot 2.99H_2O$	1.517	286.27	24.709	2.99	3.00	1.00	Hey and Bannister (1936)
129	Scolecite	$Ca_{0.363}Na_{1.400}Al_{2.138}Si_{2.863}O_{10.036} \cdot 2.06H_2O$	1.484	280.82	22.681	2.06	1.90	1.08	Hey and Bannister (1936)
130	Scolecite	$Ca_{0.038}Li_{1.875}Al_{2.188}Si_{2.900}O_{10.060} \cdot 2.04H_2O$	1.500	265.12	22.127	2.04	1.98	1.03	Hey and Bannister (1936)
131	Scolecite	$Ca_{0.975}(NH_4)_{0.063}Al_{2.163}Si_{2.863}O_{9.977} \cdot 2.58H_2O$	1.517	285.54	24.646	2.58	2.97	0.87	Hey and Bannister (1936)
132	Stellerite	$Ca_{0.945}Mg_{0.008}Sr_{0.003}Na_{0.043}K_{0.035}Al_{1.983}Fe_{0.015}Si_{7.005}O_{18} \cdot 7.03H_2O$	1.493	553.3	45.527	7.03	7.21	0.98	Galli and Passaglia (1973)
133	Tetranatrolite	$Ca_{0.412}Na_{7.044}K_{0.372}Ti_{0.012}Fe_{0.024}Al_{7.828}Si_{12.172}O_{40.252} \cdot 9.44H_2O$	1.486	1125.86	92.320	9.44	8.89	1.06	Chen and Chao (1980)

important classes of hydrous minerals and because we used mean electronic polarizability for the calculation of their total polarizabilities in contrast to the non-zeolitic minerals, where the total polarizabilities are calculated from electronic polarizabilities of cations with specific coordination numbers (CNs). Whereas the cation coordination is known for most of the non-zeolitic minerals, it is not clearly determined for most of the zeolite species where the chemical composition and the refractive indices have been determined but not the crystal structure. Therefore, Table 1 lists the results on 149 zeolites obtained with mean electronic polarizabilities, and Table S1 in the Supplement lists the results on 770 non-zeolitic minerals and synthetic compounds based on electronic polarizabilities taken from Table 4 in Shannon and Fischer (2016) for specific coordination numbers of cations. For the zeolites, the mean electronic polarizabilities of a cation in a certain oxidation state is calculated as the average of all cations of the same kind with different coordination numbers weighted by the number of entries used to determine the polarizability (see Table 4 in Shannon and Fischer, 2016). The mean values are listed in Table 2. They are internally stored in POLARIO (Fischer et al., 2018) used to calculate the water content of zeolites in Table 1. Zeolite entries are selected if they belong to one of the 237 types listed in the Database of Zeolite Structures of the International Zeolite Association (Baerlocher and McCusker, 2019). Thus, it also contains minerals like cancrinite which are not considered to be zeolite minerals but topologically have a zeolite-type framework. Only those entries are included in Table 1 where the optical data, the chemical composition, and the unit-cell parameters are available for the same specimen. There are a few exceptions where it was clear that the data from different publications can be assigned to the same crystal. We were aiming for a dataset large enough to have a representative selection and not necessarily for completeness.

All entries in Table 1 conform to the criteria listed above. However, the entries at the end of Table 1 (no. 145 to 149) show unusual deviations between observed and calculated H_2O content which are assumed to be due to uncertainties in the chemical composition. Zeolites and zeolite-type compounds having occluded anionic or neutral species also show high deviations and are listed separately in Table 3. Details are discussed below. Not considered in this compilation of hydrous minerals are compounds containing elements where the electronic polarizabilities have not been determined in Shannon and Fischer (2016). These are, for example, cations with lone-pair electrons (Tl^+, Sn^{2+}, Pb^{2+}, As^{3+}, Sb^{3+}, Bi^{3+}, S^{4+}, Se^{4+}, Te^{4+}, Cl^{5+}, Br^{5+}, and I^{5+}) which do not fit the simple scheme of additivity. Also excluded from the compilation are compounds with sterically strained structures (Gagné et al., 2018) and some compounds with corner-shared or edge-shared octahedral networks (see Shannon and Fischer, 2016; Shannon et al., 2017) showing

Table 1. Continued

No.	Zeolite name	Chem. composition[a]	<*n*>[b]	V_m (Å^3)[c]	α_{obs} (Å^3)[d]	n_w (obs)[e]	n_w (calc)[f]	n_w (obs)/ n_w (calc)[g]	References[h]
134	Tetranatrolite	$Ca_{0.188}Na_{7.144}Al_{7.684}Si_{12.316}O_{39.916} \cdot 9.00H_2O$	1.484	1126.02	90.947	9.00	9.00	1.00	Chen and Chao (1980)
135	Thomsonite	$Ca_{1.620}Na_{1.475}Al_{4.520}Si_{5.430}O_{20} \cdot 6.34H_2O$	1.514	565.0	48.483	6.34	5.41	1.17	Hey and Bannister (1932b)
136	Thomsonite	$Ca_{1.840}Na_{0.745}Al_{4.585}Si_{5.455}O_{20} \cdot 6.10H_2O$	1.523	563.3	49.187	6.10	5.87	1.04	Hey and Bannister (1932b)
137	Thomsonite	$Ca_{1.005}Na_{2.710}Al_{4.615}Si_{5.355}O_{20} \cdot 5.48H_2O$	1.528	565.0	49.809	5.48	6.56	0.84	Hey and Bannister (1932b)
138	Thomsonite	$Ca_{2.000}Na_{1.035}Al_{5.030}Si_{4.970}O_{20} \cdot 5.95H_2O$	1.534	566.7	50.528	5.95	6.43	0.93	Hey and Bannister (1932b)
139	Tschernichite	$Ca_{0.97}Na_{0.05}Mg_{0.08}Al_{2.00}Fe_{0.02}Si_{5.95}O_{16} \cdot 7.96H_2O$	1.483	518.8	41.818	7.96	7.01	1.14	Boggs et al. (1993)
140	Wairakite	$Mg_{0.005}Ca_{0.658}Na_{0.594}K_{0.014}Al_{1.800}Fe_{0.025}Si_{4.166}O_{12.037} \cdot 2.27H_2O$	1.499	316.7	26.378	2.27	1.98	1.15	Seki and Oki (1969)
141	Weinebeneite	$Ca_{0.99}Be_{3.02}P_{1.97}O_{7.88}(OH)_{2.11} \cdot 4H_2O$	1.523	276.7	24.161	4	3.7	1.08	Walter (1992)
142	Willhendersonite	$K_{0.90}Ca_{1.01}Al_{2.93}Si_{3.08}O_{12} \cdot 5.43H_2O$	1.511	403.8	34.447	5.43	5.98	0.91	Peacor et al. (1984)
143	Yugawaralite	$Mg_{0.01}Ca_{0.88}Na_{0.02}Al_{1.94}Si_{6.09}O_{16} \cdot 4.20H_2O$	1.498	441.35	36.686	4.20	4.06	1.03	Pongiluppi (1977)
144	Yugawaralite	$Mg_{0.007}Ca_{0.889}Sr_{0.012}Na_{0.013}K_{0.007}Al_{2.004}Fe_{0.004}Si_{5.993}O_{15.917} \cdot 3.93H_2O$	1.497	440.8	36.562	3.93	4.01	0.98	Eberlein et al. (1971)
145	Paulingite	$Ca_{4.20}Ba_{0.35}K_{7.00}Na_{1.40}Al_{5.60}Si_{36.40}O_{84} \cdot 50.1H_2O$	1.473	2702.7	213.285	50.1	27.4	1.83	Kamb and Oke (1960)
	Paulingite	$Ca_{3.92}Ba_{0.33}K_{6.54}Na_{1.31}Al_{5.23}Si_{36.99}O_{84} \cdot 46.7H_2O$	1.473	2702.7	213.285	46.7	28.8	1.62	
146	Pollucite	$Cs_{0.589}Na_{0.173}Li_{0.051}Rb_{0.022}K_{0.010}Ca_{0.002}Al_{0.836}Si_{2.161}O_6 \cdot 0.33H_2O$	1.517	159.80	13.793	0.33	0.57	0.58	Černý and Simpson (1978)
147	Pollucite	$Cs_{0.629}Na_{0.156}Li_{0.079}Rb_{0.022}K_{0.009}Al_{0.884}Si_{2.112}O_6 \cdot 0.27H_2O$	1.520	159.72	13.866	0.27	0.53	0.51	Černý and Simpson (1978)
148	Pollucite	$Cs_{0.630}Na_{0.114}Li_{0.053}Rb_{0.020}K_{0.006}Ca_{0.003}Mg_{0.003}Al_{0.856}Si_{2.151}O_6 \cdot 0.21H_2O$	1.523	159.72	13.947	0.21	0.61	0.34	Černý and Simpson (1978)
149	Tschörtnerite	$Ca_{5.60}Sr_{1.04}K_{0.70}Ba_{0.30}Cu_{2.90}Fe_{0.09}Al_{11.85}Si_{12.06}O_{48}(OH)_{8.44} \cdot 14.01H_2O$	1.504	1975.9	166.235	14.01	27.4	0.51	Effenberger et al. (1998)

[a] Chemical composition normalized according to the formula unit as listed in Coombs et al. (1998). [b] Mean refractive index <*n*>. [c] Molar volume V_m per formula unit. [d] Observed total electronic polarizability calculated from mean refractive index using Eq. (1). [e] Observed number of H_2O molecules per formula unit as given in the respective literature. [f] Number of H_2O molecules per formula calculated as explained in the text, using the program POLARIO (Fischer et al., 2018). [g] Factor relating the calculated to the observed H_2O content. [h] lp is lattice parameters, and RI is refractive index. [i] Chabazite with composition $Na_{0.08}K_{0.42}Ca_{0.84}Mg_{0.29}Sr_{0.03}Ba_{0.09}Al_{3.17}Fe_{0.08}Si_{8.81}O_{24} \cdot 10.84H_2O$ was omitted because of Fe_2O_3 impurities (Passaglia, 1970).

systematic deviations between observed and calculated polarizabilities.

4 Example

The approach used here is demonstrated in the example of synthetic analcime (entry 2 in Table 1) having the chemical composition $Na_{0.9}Al_{0.9}Si_{2.1}O_6 \cdot 1.1H_2O$, with data from sample 1 in Table 1 of Černý (1974). The following steps are taken to determine the water content from the refractive indices.

1. The observed total electronic polarizability α_{obs} is calculated using Eq. (1) with $V_{\mathrm{m}} = 160.71\,\text{Å}^3$ (unit-cell volume from Table 1 in Černý, 1974, $V = 2571.35\,\text{Å}^3$, divided by the number of formula units, $Z = 16$) and isotropic $n = 1.486$, yielding $\alpha_{\mathrm{obs}} = 13.034\,\text{Å}^3$.

2. The calculated total electronic polarizability α_{calc} of the anhydrous part of the chemical composition is calculated using the additivity rule with the individual electronic polarizabilities of ions from Shannon and Fischer (2016). Because the coordination number (CN) of Na is not determined in analcime (Černý, 1974), a mean value for Na with different CNs is used calculated according to $\alpha(\mathrm{Na}) = (17 \cdot 0.760 + 27 \cdot 0.650 + 207 \cdot 0.560 + 97 \cdot 0.490 + 197 \cdot 0.430 + 49 \cdot 0.380 + 25 \cdot 0.340 + 5 \cdot 0.300 + 9 \cdot 0.270)/633 = 0.489\,\text{Å}^3$, with values taken from Table 4 in Shannon and Fischer (2016). For the framework atoms Al and Si, the respective values for CN $= 4$ are used. Electronic polarizabilities and the mean values are internally stored in the program POLARIO (Fischer et al., 2018), which is used for all calculations. Thus, $\alpha_{\mathrm{calc}}(\mathrm{anhydrous}) = 0.9 \cdot \alpha(\mathrm{Na}) + 0.9 \cdot \alpha(\mathrm{Al}) + 2.1 \cdot \alpha(\mathrm{Si}) + 6 \cdot \alpha(\mathrm{O}) = 0.9 \cdot 0.489 + 0.9 \cdot 0.533 + 2.1 \cdot 0.284 + 6 \cdot 1.688 = 11.439\,\text{Å}^3$, where $\alpha(\mathrm{O})$ is calculated using Eq. (3), with $\alpha_{-}^{o} = 1.79\,\text{Å}^3$ and $N = 1.776\,\text{Å}^3$ taken from Table 5 in Shannon and Fischer (2016) and $V_{\mathrm{an}} = V_{\mathrm{m}}/6 = 26.79\,\text{Å}^3$.

3. The difference $\alpha_{\mathrm{obs}} - \alpha_{\mathrm{calc}} = 1.595\,\text{Å}^3$ represents the contribution of H_2O to the total electronic polarizability. The individual electronic polarizability of H_2O taken from Table 5 in Shannon and Fischer (2016) is $\alpha(H_2O) = 1.62\,\text{Å}^3$. However, the simple determination of the number of H_2O molecules n_w pfu according to $n_w = 1.595/1.62 = 0.98$ is not correct because n_w adds to the anion volume ($V_{\mathrm{an}} = V(\mathrm{O}) + V(H_2O) = V_{\mathrm{m}}/(n_{\mathrm{O}} + n_w)$ and thus contributes to the polarizability of the anhydrous part as well as that expressed in Eq. (4). Only the solution of Eq. (4) solved for n_w yields the correct value. This is done numerically in POLARIO, yielding 1.09 H_2O molecules pfu, which compares well with the observed 1.100 molecules determined in Černý (1974).

Alternatively, the H_2O content could be calculated using the Gladstone–Dale approach after Mandarino (1976), where the refractive index n is calculated from $n = K_c \cdot D + 1$ with $K_c = \sum_i \frac{k_i p_i}{100}$ and where k_i values are Gladstone–Dale constants, p_i values are weight percentages, and D is the density (see also Shannon and Fischer, 2016). For the example of analcime, the resulting number of H_2O molecules would be 0.89 H_2O per formula unit using Gladstone–Dale constants from Mandarino (1981) and Eggleton (1991). A detailed comparison between our polarizability approach and the Gladstone–Dale concept will be published in a follow-up paper.

5 Comparison between observed and calculated H_2O content in hydrous minerals

As mentioned above, the group of zeolite minerals was studied separately using *mean* electronic polarizabilities for the calculations. Figure 1 shows the water content calculated with Eq. (4) compared with the water content derived from analytical determinations as published in the respective references listed in Table 1. The factors relating the calculated to the observed values are shown in Fig. 2. It clearly demonstrates that the calculated values show a reasonable fit with the observed amount of H_2O, with factors $f = n_w(\mathrm{obs})/n_w(\mathrm{calc})$ being close to 1. Outliers in Figs. 1 and 2 are mainly explained by uncertainties in the determination of chemical compositions and/or refractive indices.

In paulingite (145), something must be wrong in the chemical composition. The authors state the following: "The Al/Si ratio of 0.15 given by the analysis conflicts with the cation composition ... which requires an Al/Si ratio of 0.47. Either the analysis is internally inconsistent, or else anions must be present outside the tectosilicate framework" (Kamb and Oke, 1960). The composition given in Table 1 is scaled to 42 framework cations and fixed to 84 O atoms corresponding to a factor of 3.5 relative to the original composition given in Kamb and Oke (1960), whereas 89.95 O atoms would be needed for charge compensation, which, however, does not represent a TO_2 framework. Alternatively, in the second line 145 in Table 1 the non-oxygen content is scaled down to achieve charge balance. Then the factor relating calculated and observed H_2O content changes from 1.83 to 1.62, which is lower but still rather high. In later work, Lengauer et al. (1997) investigated paulingite (94) with a different composition with 27 H_2O molecules derived from thermogravimetric analysis (TGA) and 33.5 H_2O calculated from the refractive index, yielding a factor of 0.81. The misfits for pollucite (146–148) might be due to errors in the chemical composition and/or the determination of the H_2O content. According to Beger (1969) the sum of Cs + H_2O should be equal to 1, whereas it is 0.34, for example, in pollucite (148). In tschörtnerite (149), "A quantitative determination

Figure 1. Histogram of observed (blue) and calculated (red) water content. Entries 145 to 149 are omitted (see text for explanation). The two entries with H_2O content > 50 (8 – boggsite; 69 – gottardiite) are not shown.

of H_2O/OH was not possible because of the small amount of material available" (Effenberger et al., 1998). A number of 14 molecules pfu was calculated by difference from electron microprobe analyses (EMPAs), and 20 H_2O were determined from the crystal-structure analysis. A loss of H_2O is assumed due to the high-vacuum measuring conditions in the EMPA: "A part of the total amount of H_2O is given as OH in order to achieve charge balance" (Effenberger et al., 1998). In total, this yields high uncertainties concerning the real H_2O content in tschörtnerite. The authors assume an H_2O content ≥ 20, which is much closer to the amount of 27.4 molecules calculated by us.

There are nine compounds listed in Table 3 containing anionic and/or neutral species (SO_3, SO_4, CO_2, or CO_3) oc-

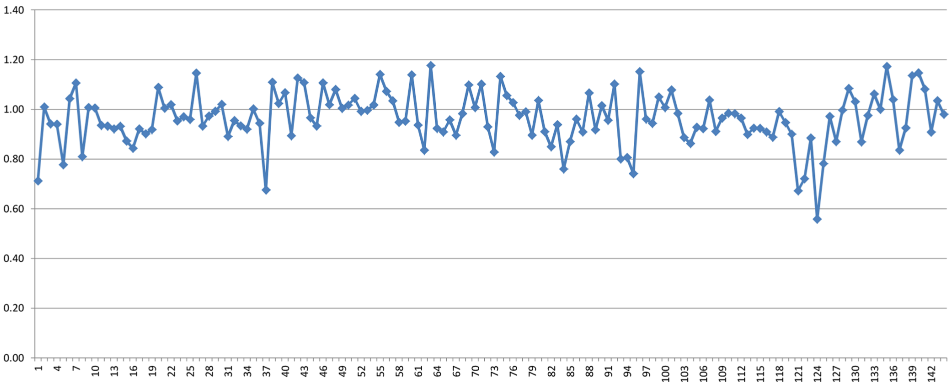

Figure 2. Plot of factors relating calculated to observed amount of H_2O in zeolite-type minerals. The sequence from left to right follows the sequence of entries in Table 1. Entries 145 to 149 are omitted (see text for explanation).

Table 2. Electronic polarizabilities α of cations from Table 4 in Shannon and Fischer (2016) averaged over different coordination numbers, including NH_4 and five H_xO_y species.

Cation	α (Å^3)	Cation	α (Å^3)	Cation	α (Å^3)	Cation	α (Å^3)
Ag^+	3.100	Fe^{2+}	2.036	Mg^{2+}	0.665	Si^{4+}	0.283
Al^{3+}	0.487	Fe^{3+}	3.854	Mn^{2+}	2.062	Sm^{3+}	3.579
As^{5+}	1.629	Ga^{3+}	1.641	Mn^{3+}	3.840	Sn^{4+}	2.910
B^{3+}	0.085	Gd^{3+}	3.516	Mo^{6+}	4.512	Sr^{2+}	2.073
Ba^{2+}	3.285	Ge^{4+}	1.625	N^{5+}	0.001	Ta^{5+}	5.200
Be^{2+}	0.165	H_3O^+	1.450	Na^+	0.489	Tb^{3+}	3.269
C^{4+}	0.001	$H_3O_2^-$	2.670	Nb^{5+}	5.780	Te^{6+}	4.430
Ca^{2+}	1.616	$H_4O_4^{4-}$	6.400	Nd^{3+}	3.796	Th^{4+}	4.395
Cd^{2+}	2.692	$H_5O_2^+$	3.100	NH^{4+}	3.180	Ti^{3+}	3.600
Ce^{3+}	3.916	$H_7O_4^-$	9.500	Ni^{2+}	1.710	Ti^{4+}	4.954
Ce^{4+}	7.157	Hf^{4+}	3.310	P^{5+}	0.036	Tm^{3+}	2.847
Cl^{7+}	0.007	Hg^+	7.000	Pr^{3+}	3.825	U^{4+}	5.000
Co^{2+}	1.725	Hg^{2+}	6.000	Pu^{4+}	4.300	V^{3+}	2.960
Cr^{3+}	3.020	Ho^{3+}	3.045	Rb^+	1.857	V^{4+}	2.627
Cr^{6+}	5.400	I^{7+}	3.075	Re^{7+}	3.200	V^{5+}	4.229
Cs^+	3.102	In^{3+}	2.520	Rh^{3+}	4.020	W^{6+}	3.879
Cu^{2+}	4.420	K^+	1.340	S^{6+}	0.011	Y^{3+}	2.757
Dy^{3+}	3.180	La^{3+}	4.057	Sb^{5+}	3.100	Yb^{3+}	2.799
Er^{3+}	3.027	Li^+	0.307	Sc^{3+}	2.308	Zn^{2+}	1.709
Eu^{2+}	3.875	Lu^{3+}	2.767	Se^{6+}	1.510	Zr^{4+}	4.103
Eu^{3+}	3.117						

cluded in the zeolite cavities. All these compounds show unusually high deviations between the observed and calculated amount of H_2O. It is apparent that these species in zeolites must be treated separately in our concept, with individual electronic polarizabilities deviating from other sulfates, sulfites, and carbonates. For liottite (156 in Table 3; Merlino and Orlandi, 1977b) the number of H_2O molecules was even calculated to be negative because the total polarizability of the anhydrous part of the compound was already higher than the corresponding observed value. However, it was shown in subsequent work by Ballirano et al. (1996) that it does not contain H_2O, which might confirm our findings in addition to the problem with the anionic species.

The mean value of the factor relating the calculated amount of H_2O to the observed one is more or less meaningless because high and low factors, each representing large errors, level each other out. More significant is the distribution of factors as shown in Fig. 3, where the bars in the histogram represent the frequency of occurrence of factors within a range of factors indicated on the horizontal axis. The mode is between 0.9 and 1.0, with 64 % of the factors between 0.9 and 1.1 and 86 % between 0.8 and 1.2.

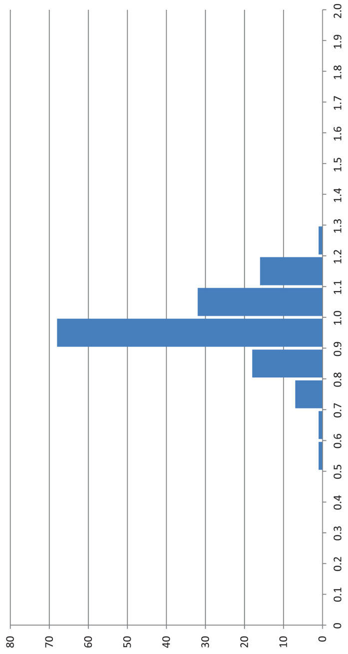

Figure 3. Frequency of occurrence of the factors for the zeolite entries 1–144 listed in Table 1 and shown in Fig. 2. **(a)** Factors calculated from polarizability analysis using different electronic polarizabilities for cations with different coordination numbers (from Table 4 in Shannon and Fischer, 2016). **(b)** Factors calculated from polarizability analysis using mean electronic polarizabilities from Table 2.

The situation is similar for the non-zeolitic minerals listed in Table S1, with 770 entries. The factors relating the calculated number of H_2O molecules to the observed ones are plotted in Fig. 4, which shows a few outliers caused by inaccuracies in the chemical compositions, difficulties in the measurement of the refractive indices, or the observed H_2O content just estimated or calculated and not determined by thermal analyses. Lotharmeyerite (entry 675) shows the largest deviation from 1 in Fig. 4a and b because of uncertainties in the observed OH (partially disordered) and H_2O content (Yang et al., 2012). Because the majority of the entries show a reasonable fit with factors close to 1, we do not discuss here specific reasons for deviations. It should be noted that these factors are calculated irrespective of the precision of the number of molecules listed in the original publications. The number of H_2O molecules for the first 30 entries in Table S1, for example, is given in integral numbers by the authors but calculated with all decimal places. If the calculated values are rounded to integers, they correspond exactly to the observed numbers except chukhrovite (27), where 12 H_2O molecules are measured and 11.28 are calculated.

Thus, there are various sources of possible deviations. This might include rounded numbers, especially for low H_2O content, where a number of 1 H_2O molecule could be anything between 0.5 and 1.5 and therefore might already represent an error of 50 %. Other sources of errors are uncertainties in the chemical compositions, especially when they are based on energy-dispersive X-ray spectroscopy (EDX) analyses, estimated and not experimentally determined H_2O content, insufficient quality of crystals for accurate measurements of the refractive indices, and also errors in our empirically determined electronic polarizabilities of cations and anions (Shannon and Fischer, 2016), which are derived in least-squares procedures. The cumulation of such errors will be reflected by factors significantly deviating from 1. Despite these in-

Table 3. Entries of zeolite-type compounds with occluded anionic species. Numbering continues to the sequence in Table 1.

No.	Zeolite name	Chem. composition	<n>	V_m (Å^3)	α_{obs} (Å^3)	n_w (obs)	n_w (calc)	n_w (obs)/ n_w (calc)	References
150	Cancrinite	$Na_{6.89}Ca_{0.12}Mg_{0.03}K_{0.02}Si_{7.20}Al_{4.90}O_{24.02}(CO_3)_{1.10}(SO_4)_{0.04} \cdot 2.79H_2O$	1.503	699.10	58.699	2.79	3.73	0.75	Khomyakov et al. (1991a) cited in Jambor and Grew (1993)
151	Cancrisilite	$Na_{6.70}K_{0.08}Ca_{0.09}Fe_{0.05}Mg_{0.03}Al_{4.79}Si_{7.21}O_{24.26}(CO_3)_{0.91} \cdot 3.20H_2O$	1.503	699.1	58.699	3.20	4.20	0.76	Khomyakov et al. (1991b)
152	Carbobystrite	$Na_{7.40}K_{0.38}Al_{6.04}Si_{6.02}O_{24}(CO_3) \cdot 3.5H_2O$	1.496	718.5	59.482	3.5	4.09	0.86	Khomyakov et al. (2010)
153	Depmeierite	$Na_{7.58}K_{0.12}Si_{6.19}Al_{5.81}O_{24}(PO_4)_{0.47}(CO_3)_{0.22}(OH)_{0.02}(SO_4)_{0.01} \cdot 3.35H_2O$	1.496	729.4	60.385	3.35	5.18	0.65	Pekov et al. (2011)
154	Farneseite	$Na_{36.43}K_{9.18}Ca_{8.75}Si_{42.50}Al_{41.50}O_{168}(SO_4)_{11.43}F_{0.16}Cl_{0.48} \cdot 3.03H_2O$	1.500	5315.54	443.631	3.03	9.5	0.32	Cámara et al. (2005)
155	Franzinite	$Na_{21.53}K_{5.22}Ca_{12.50}Mg_{0.20}Fe_{0.08}Si_{31.32}Al_{28.68}O_{120}(SO_4)_{7.72}(CO_3)_{2.03}(OH)_{3.46}Cl_{0.59} \cdot 4.31H_2O$	1.511	3821.1	325.966	4.31	0.55	7.84	Merlino and Orlandi (1977a)
156	Liottite	$Ca_{10.76}Na_{9.29}K_{3.82}Al_{17.66}Fe_{0.16}Si_{18.34}O_{72}(SO_4)_{3.91}(CO_3)_{1.72}Cl_{2.61}(OH)_{3.58} \cdot 1.83H_2O$	1.529	2298.2	202.984	1.83	0	0.00	Merlino and Orlandi (1977b)
157	Marinellite	$Na_{31.86}K_{11.13}Ca_{6.06}Al_{36.02}Si_{35.98}O_{144.6}(SO_4)_{8.12}Cl_{1.62} \cdot 3.41H_2O$	1.496	4563.1	377.762	3.41	7.98	0.43	Bonaccorsi and Orlandi (2003)

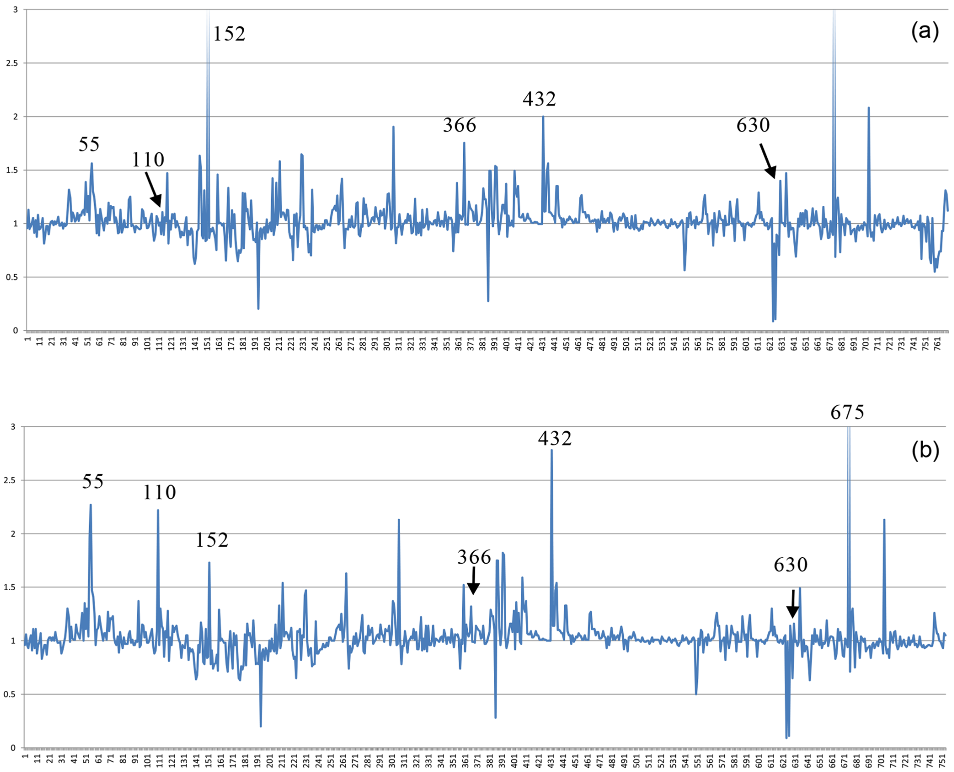

Figure 4. Plot of factors relating calculated to observed amount of H_2O in non-zeolitic minerals. The sequence from left to right follows the sequence of entries in Table S1.

fluences, the data shown in Figs. 1 to 5 clearly show that there is on average a very good fit between the observed and calculated amount of H_2O. In general the best results are achieved using the individual electronic polarizabilities of cations with specific coordination numbers (Table 4 in Shannon and Fischer, 2016). However, mean polarizabilities (Table 2) yield results that are sufficiently accurate if the CN of cations has not been determined. This is shown in Fig. 4, comparing the two approaches yielding essentially similar results with a few outliers. Entries 55 (priceite), 110 (calcioancylite-Nd), and 432 (bassanite), for example, have factors much higher for mean polarizabilities, but entries 152 (milarite), 366 ($Li_2SO_4 \cdot H_2O$), and 630 (martyite), for example, have factors closer to 1 as compared with the corresponding values from the individual polarizabilities. Generally we recommend verifying questionable results derived from mean polarizability with corresponding calculations using the CN-dependent polarizabilities.

6 Conclusions

The evaluation of 927 hydrous minerals and inorganic compounds showed that their H_2O content can be calculated from their mean refractive indices if the anhydrous part of the chemical composition is known. Thus, single crystals with dimensions < 100 µm, usually used in X-ray diffraction analyses, can be used to determine the number of H_2O molecules per formula unit if higher amounts of the sample are not available for thermal analyses. Based on the excellent overall agreement between the observed and calculated H_2O contents of 157 zeolites and 770 other hydrates and the unusual deviations of paulingite, pollucite, tschörtnerite, liottite, and lotharmeyerite, we suggest that when strong disagreements

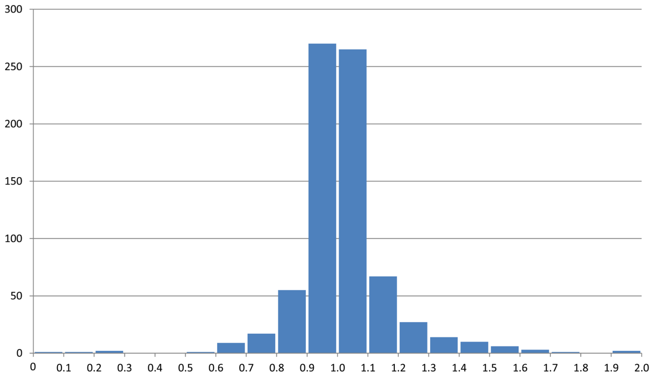

Figure 5. Frequency of occurrence of the factors for the non-zeolite entries listed in Table S1 and shown in Fig. 4. The three outliers with factors > 2 are omitted.

occur, the refractive index, composition, and/or crystal structure should be more carefully investigated.

Code availability. The program POLARIO (Fischer et al., 2018) calculates the mean refractive index from the chemical composition and the molar volume. It also determines the H_2O content of hydrous minerals from the anhydrous part of the chemical composition. The program can be downloaded free of charge from https://www.brass.uni-bremen.de/ (Fischer et al., 2018). Version 1.1 of the program was uploaded to the website on 23 October 2018.

Supplement. The supplement related to this article is available online at: https://doi.org/10.5194/ejm-32-27-2020-supplement.

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