

Introduction

1 General remarks

Up to June 2006, 167 zeolite framework types have been approved by the Structure Commission of the International Zeolite Association (IZA), 109 of which are now covered in this series. Since volume C [2002Bau1] went to press, we have added about 700 structures to our data base now containing 4,200 entries of zeolite-type structures (that is much more than one can get from the most extensive database for inorganic crystal structures [2005ICS1] which produces 1502 hits for the keyword “zeolites” in the Mineral/Group search option). The chapters on codes ASV, BCT, BEC, CDO, EON, ETR, GIU, IHW, ITH, ITW, IWR, IWW, and LIT will be published together with additional entries for previously covered codes at the end of the last volume of this series.

In this volume D, 1140 crystal structure determinations, refinements, and descriptions are listed, dominated by the large numbers of LTA-type structures (375 entries) representing one of the most important ion exchange materials especially in detergents (LTA.6.1), followed by NAT-type structures (236) and RHO-type structures (160). The natrolite minerals (NAT) and RHO-type zeolites are interesting materials for crystal chemical studies because of their extremely flexible framework structures. Zeolite rho is an important catalyst for the selective synthesis of dimethylamines (RHO.6). Even more interesting are the MFI-type zeolites listed with 116 entries which are used in petrochemical processes (see MFI.6).

The standardization of atomic coordinates according to a systematic-subgroup relation is one of the special goals of this work described in chapter 3 of volume B. Details on the standardization process are published in [2004Fis1] and its benefits for crystal chemical comparisons are demonstrated in [2004Bau1].

Errors found by us in volumes A, B, and C or communicated to us before this volume went to press are listed under Errata at the end of this volume. Updates to all codes, especially new symmetry derivations, chemical data, and structural parameters will be given in or after the last volume of this series.

As described in chapter 1 of volume B, all crystal structure entries have been checked for their internal and external consistency. Misprints in the original literature were corrected, partly after correspondence with the authors, and partly to the best of our knowledge, especially if typographical errors were obvious or in all those cases where the authors either did not respond to our inquiries or could not resolve the problem.

2 Systematics, descriptions, and definitions

2.1 Modifications and changes

2.1.1 Bärnighausen tree

Starting in this volume D we have assigned the letter *i* to *klassengleich* subgroup relationships with identical space groups in the Bärnighausen trees (see, e.g., NAT p. 273). The derivations of the symmetry relationships were greatly facilitated making use of [2004Won1].

2.1.2 Chemical composition

Chemical compositions are still given in the format described in chapter 10.2 of volume B [2000Bau1] with cations on the left and neutral species and anions right on the right of the framework compositions separated by periods. However, it should be noted that we do not distinguish between cationic and neutral molecules in the sorbate/template column of Tables FTC.2.1 (FTC = framework type code). Ammonium (NH_4^+) is never listed as a sorbate because it is too small and similar to K^+ . Larger molecules like its methylamine derivatives are listed though.

2.1.3 Crystal structure drawings

Starting with this volume D we use a new version of the STRUPLO program (latest release from [2006Fis1]) for the crystal structure drawings. It is now capable of drawing solid isometric cages.

2.2 Minerals with zeolite-type frameworks

Mineral names in Tables FTC.1.1 are given in square brackets when the minerals were modified by dehydration, calcination, or cation exchange. The mineral name refers to the original species even though its chemical composition might be changed by cation exchange, thermal or acid treatment. The names are given in parentheses if it is a synthetic analogue to the mineral species. Table 2.2.1 lists all entries of Table 2.3.1 of volume B and Table 2.2.1 of volume C together with the new entries of this volume.

Table 2.2.1 Selected entries of minerals with framework type codes ABW to RHO).

mineral name	chemical composition	space group	FD	entry code
afghanite	$\text{Na}_{18}\text{Ca}_{10}\text{K}_{0.8} \cdot \text{Al}_{24}\text{Si}_{24}\text{O}_{96} \cdot 10.4\text{H}_2\text{O}$ $0.8\text{CO}_3 \ 5.6\text{Cl} \ 5.6\text{SO}_4$	$P6_3mc$	15.9	AFG1991a01
	$\text{Na}_{18}\text{Ca}_{10}\text{K}_4 \cdot \text{Al}_{24}\text{Si}_{24}\text{O}_{96} \cdot 6\text{SO}_4 \cdot 6\text{Cl}$	$P31c$	15.8	AFG1997a01
amicite	$\text{K}_4\text{Na}_4 \cdot \text{Al}_8\text{Si}_8\text{O}_{32} \cdot 10\text{H}_2\text{O}$	$I112$	15.2	GIS1979a01
ammonioleucite	$(\text{NH}_4)_{14} \cdot \text{Al}_{14}\text{Si}_{34}\text{O}_{96}$	$I4_1/a$	20.0	ANA1998e01
analcime	$\text{Na}_{16} \cdot \text{Al}_{16}\text{Si}_{32}\text{O}_{96} \cdot 16\text{H}_2\text{O}$	$Ia\bar{3}d$	18.5	ANA1972a01
	$\text{Na}_{16} \cdot \text{Al}_{16}\text{Si}_{32}\text{O}_{96} \cdot 16\text{H}_2\text{O}$	$I4_1/a cd$	18.6	ANA1978a05
	$\text{Na}_{16} \cdot \text{Al}_{16}\text{Si}_{32}\text{O}_{96} \cdot 16\text{H}_2\text{O}$	$Ibca$	18.6	ANA1978a04
bellbergite	$(\text{Ca},\text{Na})_4\text{Ca}_2\text{Sr}_2(\text{K},\text{Ba})_2 \cdot \text{Al}_{18}\text{Si}_{18}\text{O}_{72}$ $\cdot 30\text{H}_2\text{O}$	$P6_3/mmc$	14.8	EAB1993a01
bikitaite	$\text{Li}_2 \cdot \text{Al}_2\text{Si}_4\text{O}_{12} \cdot 2\text{H}_2\text{O}$	$P12_11$	20.3	BIK1974a01

Table 2.2.1 (continued)

mineral name	chemical composition	space group	FD	entry code
boggsite	$\text{Li}_2 \cdot \text{Al}_2\text{Si}_4\text{O}_{12} \cdot 2\text{H}_2\text{O}$	$P 1$	20.3	BIK1986a01
	$\text{Ca}_{7.8}\text{Na}_{2.9}\text{Al}_{18.5}\text{Si}_{77.5}\text{O}_{192} \cdot 70\text{H}_2\text{O}$	$I m m a$	15.6	BOG1990a01
	$\text{Sr}_{1.5}\text{Ba}_{0.5} \cdot \text{Al}_4\text{Si}_{12}\text{O}_{32} \cdot 10\text{H}_2\text{O}$	$P 2_1/m$	17.3	BRE1977a01
brewsterite	$\text{SrBa} \cdot \text{Al}_4\text{Si}_{12}\text{O}_{32} \cdot 10\text{H}_2\text{O}$	$P \bar{1}$	17.4	BRE1996a02
	$\text{Na}_{10}\text{K}_4\text{Ca}_2 \cdot \text{Al}_{11.7}\text{Si}_{12.3}\text{O}_{48} \cdot 2.8\text{S}_3 \cdot 2\text{H}_2\text{O}$	$P 3 1 c$	15.7	LOS1991a01
cancrinite	$\text{Na}_6 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 1.5\text{Ca} \cdot 1.6\text{CO}_3 \cdot 2\text{H}_2\text{O}$	$P 6_3$	17.1	CAN1982b01
	$\text{Na}_7 \cdot \text{Al}_5\text{Si}_7\text{O}_{24} \cdot \text{CO}_3 \cdot 3\text{H}_2\text{O}$	$P 6_3 m c$	17.2	CAN1991d01
chabazite-Ca	$\text{Ca}_{1.95} \cdot \text{Al}_{3.9}\text{Si}_{8.1}\text{O}_{24} \cdot 13\text{H}_2\text{O}$	$R \bar{3} m$	14.5	CHA1963a01
	$\text{Ca}_{1.4}\text{K}_{0.2}\text{Mg}_{0.4}\text{Sr}_{0.3} \cdot \text{Al}_{3.9}\text{Si}_{8.2}\text{O}_{24} \cdot 12.2 \text{H}_2\text{O}$	$R \bar{3} m$	14.4	CHA1982b01
	$\text{Ca}_{1.4}\text{Sr}_{0.3} \cdot \text{Al}_{3.8}\text{Si}_{8.3}\text{O}_{24} \cdot 13\text{H}_2\text{O}$	$R \bar{3} m$	14.5	CHA1982c01
	$\text{Ca}_{1.4}\text{K}_{0.2}\text{Na}_{0.3} \cdot \text{Al}_{3.4}\text{Si}_{8.6}\text{O}_{24} \cdot 13\text{H}_2\text{O}$	$R \bar{3} m$	14.6	CHA1983b01
	$\text{Ca}_{0.8}\text{Fe}_{0.6} \cdot \text{Al}_3\text{Si}_9\text{O}_{24} \cdot 10\text{H}_2\text{O}$	$R \bar{3} m$	14.5	CHA1985c02
	$\text{Ca}_{1.4}\text{K}_{0.2}\text{Na}_{0.3} \cdot \text{Al}_{3.4}\text{Si}_{8.6}\text{O}_{24} \cdot 13\text{H}_2\text{O}$	$P \bar{1}$	14.6	CHA1983b02
chabazite-Li	$\text{Ca}_{0.2}\text{Li}_{3.3} \cdot \text{Al}_{3.7}\text{Si}_{8.3}\text{O}_{24} \cdot 12\text{H}_2\text{O}$	$R \bar{3} m$	14.7	CHA1994c01
chiavennite	$\text{Ca}_4\text{Mn}_4\text{H}_8 \cdot \text{Be}_8\text{Si}_{20}\text{O}_{60} \cdot 8\text{H}_2\text{O}$	$P n a b$	20.9	CHI1995a01
clinoptilolite-Ca	$\text{Ca}_{1.9}\text{K}_{1.1}\text{Na}_{1.8} \cdot \text{Al}_{6.7}\text{Si}_{29.2}\text{O}_{72} \cdot 24\text{H}_2\text{O}$	$C 2/m$	17.1	HEU1977a01
clinoptilolite-K	$\text{Ca}_{1.1}\text{K}_{2.4}\text{Mg}_{0.3}\text{Na}_{1.2} \cdot \text{Al}_{6.6}\text{Si}_{29.5}\text{O}_{72} \cdot 18\text{H}_2\text{O}$	$C 2/m$	19.0	HEU1999c02
clinoptilolite-Na	$\text{Ca}_{1.3}\text{K}_{1.0}\text{Na}_{3.2} \cdot \text{Al}_{7.4}\text{Si}_{28.4}\text{O}_{72} \cdot 22\text{H}_2\text{O}$	$C 2/m$	17.1	HEU1975a02
dachiardite	$(\text{Na}, \text{K}, \text{Ca}_{0.5})_5\text{Al}_5\text{Si}_{19}\text{O}_{48} \cdot 13\text{H}_2\text{O}$	$C 2/m$	17.5	DAC1990a01
davyne	$\text{Na}_4\text{K}_2\text{Ca}_2 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 2\text{Cl} \cdot \text{SO}_4$	$P 6_3/m$	16.0	CAN1990a01
edingtonite	$\text{Na}_6\text{Ca}_2 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 2\text{Cl} \cdot 2\text{OH}$	$P 6_3$	15.7	CAN1990b01
	$\text{Ba}_2 \cdot \text{Al}_4\text{Si}_6\text{O}_{20} \cdot 7\text{H}_2\text{O}$	$P \bar{4} 2_1 m$	16.7	EDI1984a01
epistilbite	$\text{Ba}_2 \cdot \text{Al}_4\text{Si}_6\text{O}_{20} \cdot 8\text{H}_2\text{O}$	$P 2_1 2_1 2$	16.6	EDI1976a01
	$\text{Ca}_3\text{Na} \cdot \text{Al}_6\text{Si}_{18}\text{O}_{48} \cdot 16\text{H}_2\text{O}$	$C 1 2/m 1$	17.6	EPI1967a01
	$\text{Ca}_{2.6}\text{Na}_{0.8} \cdot \text{Al}_6\text{Si}_{18}\text{O}_{48} \cdot 16\text{H}_2\text{O}$	$C 1 2 1$	17.7	EPI1985a02
	$\text{Ca}_{2.7}\text{Na}_{0.3} \cdot \text{Al}_6\text{Si}_{18}\text{O}_{48} \cdot 16\text{H}_2\text{O}$	$C 1$	17.7	EPI1996a01
erionite-Ca	$\text{Ca}_{4.3}\text{K}_{2.2}\text{Na}_{0.2} \cdot \text{Al}_{11}\text{Si}_{25}\text{O}_{72} \cdot 36\text{H}_2\text{O}$	$P 6_3/m m c$	15.5	ERI1998a02
erionite-K	$\text{Ca}_{1.3}\text{K}_{2.0}\text{Mg}_{0.6}\text{Na}_{1.9} \cdot \text{Al}_9\text{Si}_{26}\text{O}_{72} \cdot 10\text{H}_2\text{O}$	$P 6_3/m m c$	15.6	ERI1973a01
erionite-Mg, K	$\text{Ca}_{0.7}\text{K}_{2.1}\text{Mg}_{2.4}\text{Na}_{1.3} \cdot \text{Al}_{13.1}\text{Si}_{23.6}\text{O}_{72} \cdot 27.4\text{H}_2\text{O}$	$P 6_3/m m c$	16.0	ERI1967a01
faujasite-Na	$\text{Ca}_{14}\text{Na}_{29} \cdot \text{Al}_{58}\text{Si}_{134}\text{O}_{384} \cdot 263\text{H}_2\text{O}$	$F d \bar{3} m$	12.7	FAU1964a01
ferrierite-Mg	$\text{Na}_{1.3}\text{K}_{0.2}\text{Mg}_2 \cdot \text{Al}_{5.5}\text{Si}_{30.5}\text{O}_{72} \cdot 18\text{H}_2\text{O}$	$I m m m$	17.8	FER1966a01
ferrierite-Na	$\text{Na}_3\text{KMg}_{0.5} \cdot \text{Al}_5\text{Si}_{31}\text{O}_{72} \cdot 18\text{H}_2\text{O}$	$P 1 2_1/n 1$	18.0	FER1985a01
franzinite	$(\text{Na}, \text{K})_{30}\text{Ca}_{10} \cdot \text{Si}_{30}\text{Al}_{30}\text{O}_{120} \cdot 10\text{SO}_4 \cdot 2\text{H}_2\text{O}$	$P \bar{3} m 1$	15.6	FRA2000a01
garronite	$\text{Ca}_3 \cdot \text{Al}_6\text{Si}_{10}\text{O}_{32} \cdot 14\text{H}_2\text{O}$	$I \bar{4} m 2$	15.8	GIS1992a01
	$\text{Ca}_3 \cdot \text{Al}_6\text{Si}_{10}\text{O}_{32} \cdot 14\text{H}_2\text{O}$	$I 1 1 2/b$	16.0	GIS1999c01
gismondine	$\text{Ca}_4 \cdot \text{Al}_8\text{Si}_8\text{O}_{32} \cdot 16\text{H}_2\text{O}$	$P 1 1 2_1/a$	15.3	GIS1963a01
	$\text{Ca}_8 \cdot \text{Al}_{16}\text{Si}_{16}\text{O}_{64} \cdot 16\text{H}_2\text{O}$	$P 2_1 2_1 2_1$	18.6	GIS1993a02
gmelinite-Na	$\text{Na}_8 \cdot \text{Al}_8\text{Si}_{16}\text{O}_{48} \cdot 22\text{H}_2\text{O}$	$P 6_3/m m c$	14.6	GME1982a01
gmelinite-Ca	$\text{Ca}_{2.06}\text{K}_{0.11}\text{Na}_{0.78}\text{Sr}_{1.35} \cdot \text{Al}_{7.82}\text{Si}_{16.21}\text{O}_{48} \cdot 23.23\text{H}_2\text{O}$	$P 6_3/m m c$	14.6	GME1982a02
gmelinite-K	$\text{K}_3\text{Ca}_2 \cdot \text{Al}_8\text{Si}_{16}\text{O}_{48} \cdot 24\text{H}_2\text{O}$	$P 6_3/m m c$	14.6	GME1990a01
gobbinsite	$\text{Ca}_{0.6}\text{Na}_{4.3} \cdot \text{Al}_{5.6}\text{Si}_{10.4}\text{O}_{32} \cdot 12\text{H}_2\text{O}$	$P n m 2_1$	15.9	GIS1994a01
	$\text{Ca}_{0.6}\text{K}_{2.2}\text{Na}_{2.6} \cdot \text{Al}_6\text{Si}_{10}\text{O}_{32} \cdot 12\text{H}_2\text{O}$	$P n m 2_1$	15.9	GIS1985b01
gonnardite	$\text{Na}_{4.51}\text{Ca}_{1.84} \cdot \text{Al}_{8.59}\text{Si}_{11.50}\text{O}_{40} \cdot 12.61\text{H}_2\text{O}$	$I \bar{4} 2 d$	17.2	NAT1999b01

Table 2.2.1 (continued)

mineral name	chemical composition	space group	FD	entry code
goosecreekite	$\text{Ca} \cdot \text{Al}_2\text{Si}_6\text{O}_{16} \cdot 5\text{H}_2\text{O}$	$P 1 1 2_1$	17.6	GOO1986a01
gottardiite	$\text{Ca}_{4.8}\text{K}_{0.2}\text{Mg}_{3.1}\text{Na}_{2.5} \cdot \text{Al}_{18.8}\text{Si}_{117.2}\text{O}_{272} \cdot 93\text{H}_2\text{O}$	$C c m e$	17.4	NES1996a01
harmotome	$\text{Ca}_{0.5}\text{Ba}_2 \cdot \text{Al}_5\text{Si}_{11}\text{O}_{32} \cdot 12\text{H}_2\text{O}$	$P 1 2_1/m 1$	16.0	PHI1974a02
heulandite-Ca	$\text{Ca}_{3.7}\text{Na}_{1.30} \cdot \text{Al}_{8.9}\text{Si}_{27.1}\text{O}_{72} \cdot 21\text{H}_2\text{O}$	$C 2/m$	17.2	HEU1994a01
	$\text{Ca}_{3.6}\text{K}_{0.4}\text{Na}_{1.3} \cdot \text{Al}_{9.4}\text{Si}_{26.7}\text{O}_{72} \cdot 26\text{H}_2\text{O}$	$C m$	17.1	HEU1972a02
hsianghualite	$\text{Ca}_{24}\text{Li}_{16} \cdot \text{Be}_{24}\text{Si}_{24}\text{O}_{96} \cdot 16\text{F}$	$I 2_1 3$	22.5	ANA1991c01
kalborsite	$\text{K}_6 \cdot \text{Al}_4\text{Si}_6\text{O}_{20} \cdot \text{B}(\text{OH})_4 \text{Cl}$	$P 4 2_1 c$	15.8	EDI1980a01
laumontite	$\text{Ca}_4 \cdot \text{Al}_8\text{Si}_{16}\text{O}_{48} \cdot 17.2\text{H}_2\text{O}$	$C 1 2/m 1$	17.6	LAU1992a01
H ₂ O-poor laumontite	$\text{Ca}_4 \cdot \text{Al}_8\text{Si}_{16}\text{O}_{48} \cdot 12\text{H}_2\text{O}$	$C 1 2/m 1$	17.6	LAU1970a01
Na,K-rich laumontite	$\text{Ca}_2\text{K}_2\text{Na}_2 \cdot \text{Al}_8\text{Si}_{16}\text{O}_{48} \cdot 14\text{H}_2\text{O}$	$C 1 2/m 1$	17.8	LAU2000a01
Na,K-rich laumontite	$\text{Ca}_{2.6}\text{K}_{1.6}\text{Na}_{1.2} \cdot \text{Al}_8\text{Si}_{16}\text{O}_{48} \cdot 14\text{H}_2\text{O}$	$P 1 2/a 1$	17.8	LAU1997a01
leucite	$\text{K}_{16} \cdot \text{Al}_{16}\text{Si}_{32}\text{O}_{96}$	$I 4_1/a$	20.4	ANA1976a01
	$\text{K}_{16} \cdot \text{Al}_{16}\text{Si}_{32}\text{O}_{96}$	$I a \bar{3} d$	19.4	ANA1993b05
	$\text{K}_{16} \cdot \text{Al}_{16}\text{Si}_{32}\text{O}_{96}$	$I 4_1/a c d$	19.4	ANA1990b12
levyne-Ca	$\text{Ca}_8\text{Na}_2\text{K} \cdot \text{Al}_{19}\text{Si}_{35}\text{O}_{108} \cdot 50\text{H}_2\text{O}$	$R \bar{3} m$	15.2	LEV1975a01
levyne-Na	$\text{Ca}_{3.2}\text{KNa}_{10.7} \cdot \text{Al}_{18.8}\text{Si}_{35.3}\text{O}_{108} \cdot 44.2\text{H}_2\text{O}$	$R \bar{3} m$	15.4	LEV1996a01
liottite	$\text{Ca}_{11}\text{Na}_9\text{K}_4 \cdot \text{Al}_{18}\text{Si}_{18}\text{O}_{72} \cdot 2\text{H}_2\text{O} \cdot 4\text{SO}_4 \cdot 2\text{CO}_3 \cdot 3\text{Cl} \cdot 4\text{OH}$	$P \bar{6} m 2$	15.6	LIO1977a01
	$\text{Ca}_9\text{Na}_{10}\text{K}_5 \cdot \text{Al}_{18}\text{Si}_{18}\text{O}_{72} \cdot 5\text{SO}_4 \cdot 3.5\text{Cl} \cdot 0.5\text{F}$	$P \bar{6}$	15.6	LIO1996a01
lithosite	$\text{K}_{12}\text{H}_4 \cdot \text{Al}_8\text{Si}_{16}\text{O}_{52}$	$P 1 2_1 1$	18.3	LIT1986a01
lovdarite	$\text{K}_4\text{Na}_{12} \cdot \text{Be}_8\text{Si}_{28}\text{O}_{72} \cdot 18\text{H}_2\text{O}$	$P c 2 m$	18.3	LOV1990a01
maricopaite	$\text{Ca}_{2.2}\text{Pb}_{7.2} \cdot \text{Al}_{11.6}\text{Si}_{36.4}\text{O}_{99.6} \cdot 31.8\text{H}_2\text{O}$	$C m 2 m$	16.6	MOR1994b01
marinellite	$\text{Na}_{32}\text{K}_{11}\text{Ca}_6 \cdot \text{Al}_{36}\text{Si}_{36}\text{O}_{144} \cdot 8\text{SO}_4 \cdot 1.6\text{Cl} \cdot 3.4\text{H}_2\text{O}$	$P 3 1 c$	15.8	MAR2003a01
mazzite-Mg	$\text{Ca}_{1.4}\text{K}_{2.5}\text{Mg}_{2.1}\text{Na}_{0.3} \cdot \text{Al}_{9.9}\text{Si}_{26.5}\text{O}_{72} \cdot 28\text{H}_2\text{O}$	$P 6_3/m m c$	16.1	MAZ1975a01
mazzite-Na	$\text{Na}_8 \cdot \text{Al}_8\text{Si}_{28}\text{O}_{72} \cdot 30\text{H}_2\text{O}$	$P 6_3/m m c$	16.1	MAZ2005a01
melanophlogite	$\text{Si}_{184}\text{O}_{368} \cdot 7.2\text{CH}_4 \cdot 4.08\text{CO}_2 \cdot 14.16\text{N}_2$	$P 4_2/n b c$	19.1	MEP2001a01
	$\text{Si}_{46}\text{O}_{92} \cdot 1.8\text{CH}_4 \cdot 1.02\text{CO}_2 \cdot 3.54\text{N}_2$	$P m \bar{3} n$	19.0	MEP1983a01
merlinoite	$\text{K}_5\text{Ca}_2 \cdot \text{Al}_9\text{Si}_{23}\text{O}_{64} \cdot 24\text{H}_2\text{O}$	$I m m m$	16.0	MER1979a01
mesolite	$\text{Na}_{15.92}\text{Ca}_{16.32} \cdot \text{Al}_{48.00}\text{Si}_{71.84}\text{O}_{240} \cdot 64\text{H}_2\text{O}$	$F d d 2$	17.6	NAT2000c01
microsommitte	$\text{Na}_4\text{K}_2\text{Ca}_2 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 0.9\text{SO}_4 \cdot 2.2\text{Cl}$	$P 6_3/m$	15.6	CAN1995a02
	$\text{Na}_4\text{K}_2\text{Ca}_2 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 0.9\text{SO}_4 \cdot 2.2\text{Cl}$	$P 6_3$	15.9	CAN1995a01
montesommaite	$\text{K}_5 \cdot \text{Al}_5\text{Si}_{11}\text{O}_{32} \cdot 5\text{H}_2\text{O}$	$I 4_1/a m d$	18.1	MON1990a02
mordenite	$\text{Ca}_{1.89}\text{K}_{0.14}\text{Mg}_{0.09}\text{Na}_{3.51} \cdot \text{Al}_{7.4}\text{Fe}_{0.03}\text{Si}_{40.53}\text{O}_{96} \cdot 27.26\text{H}_2\text{O}$	$C m c m$	17.2	MOR2003a01
mutinaite	$\text{Ca}_{3.8}\text{K}_{0.1}\text{Mg}_{0.2}\text{Na}_{2.8} \cdot \text{Al}_{11.2}\text{Si}_{84.9}\text{O}_{192} \cdot 60\text{H}_2\text{O}$	$P n m a$	17.6	MFI1997a01
nabesite	$\text{Na}_8 \cdot \text{Be}_4\text{Si}_{16}\text{O}_{40} \cdot 16\text{H}_2\text{O}$	$P 2_1 2_1 2_1$	16.9	NAB2002a01
natrolite	$\text{Na}_{16} \cdot \text{Al}_{16}\text{Si}_{24}\text{O}_{80} \cdot 16\text{H}_2\text{O}$	$F d d 2$	17.8	NAT1993b01
offretite	$\text{KCaMg} \cdot \text{Al}_5\text{Si}_{13}\text{O}_{36} \cdot 18\text{H}_2\text{O}$	$P \bar{6} m 2$	15.4	OFF1996a01
pahasapaite	$\text{Li}_{11.6}\text{Ca}_{5.5}\text{K}_{1.2}\text{Na}_{0.2} \cdot \text{Be}_{24}\text{P}_{24}\text{O}_{96} \cdot 38\text{H}_2\text{O}$	$I 2 3$	18.3	RHO1989c01
paranatrolite	$\text{Na}_{15.04}\text{K}_{1.76}\text{Ca}_{0.48} \cdot \text{Al}_{17.92}\text{Si}_{22.08}\text{O}_{80} \cdot 24.8\text{H}_2\text{O}$	$F 1 d 1$	16.7	NAT2004a01

Table 2.2.1 (continued)

mineral name	chemical composition	space group	FD	entry code
parthéite	$\text{Ca}_8 \cdot \text{Al}_{16}\text{Si}_{16}\text{O}_{68}\text{H}_8 \cdot 16\text{H}_2\text{O}$	$C\ 12/c\ 1$	18.2	PAR1984a01
paulingite-K	$\text{K}_{68}\text{Ba}_{1.5}\text{Ca}_{36}\text{Na}_{13} \cdot \text{Al}_{152}\text{Si}_{520}\text{O}_{1344} \cdot 705\text{H}_2\text{O}$	$Im\ \bar{3}\ m$	15.5	PAU1966a01
paulingite-Ca	$\text{Ba}_2\text{Ca}_{59}\text{K}_{36}\text{Na}_{14} \cdot \text{Al}_{173}\text{Si}_{499}\text{O}_{1344} \cdot 550\text{H}_2\text{O}$	$Im\ \bar{3}\ m$	15.5	PAU1996a01
barian	$\text{Ba}_{22}\text{Ca}_{41}\text{Fe}_{0.5}\text{K}_{36}\text{Mg}_{0.6}\text{Mn}_{0.2}\text{Na}_6 \cdot$	$Im\ \bar{3}\ m$	15.5	PAU1997a01
paulingite-Ca	$\text{Al}_{185}\text{Si}_{489}\text{Sr}_2\text{O}_{1344} \cdot 434\text{H}_2\text{O}$			
perialite	$\text{K}_8\text{Ti}_4 \cdot \text{Al}_{12}\text{Si}_{24}\text{O}_{72} \cdot 20\text{H}_2\text{O}$	$P\ 6/m\ m\ m$	16.1	LTL1990a01
phillipsite-K	$\text{Ca}_{1.7}\text{K}_{2.0}\text{Na}_{0.4} \cdot \text{Al}_{5.3}\text{Si}_{10.6}\text{O}_{32} \cdot 12\text{H}_2\text{O}$	$P\ 1\ 2_1/m\ 1$	15.8	PHI1974a01
pitiglianoite	$\text{Na}_{18}\text{K}_6 \cdot \text{Al}_{18}\text{Si}_{18}\text{O}_{72} \cdot 3\text{SO}_4\ 6\text{H}_2\text{O}$	$P\ 6_3$	16.3	CAN1991c01
pollucite	$\text{Cs}_{10}\text{Na}_3 \cdot \text{Al}_{14}\text{Si}_{34}\text{O}_{96} \cdot 4.5\text{H}_2\text{O}$	$Ia\ \bar{3}\ d$	18.8	ANA1995a01
	$\text{Cs}_{13}\text{Na}_2 \cdot \text{Al}_{15}\text{Si}_{33}\text{O}_{96} \cdot 32\text{H}_2\text{O}$	$I4_1/a\ c\ d$	18.7	ANA1995a02
quadridavyne	$\text{Na}_{16}\text{K}_4\text{Ca}_8 \cdot \text{Al}_{24}\text{Si}_{24}\text{O}_{96} \cdot 16\text{Cl}$	$P\ 6_3/m$	15.5	CAN1994a01
roggianite	$\text{Ca}_{16} \cdot \text{Be}_8(\text{OH})_{16}\text{Al}_{16}\text{Si}_{32}\text{O}_{104} \cdot 19\text{H}_2\text{O}$	$I4/m\ c\ m$	18.2	RON1991a01
scolecite	$\text{Ca}_8 \cdot \text{Al}_{16}\text{Si}_{24}\text{O}_{80} \cdot 24\text{H}_2\text{O}$	$F\ 1\ d\ 1$	17.5	NAT1997a01
tetranatrolite	$\text{Na}_{5.85}\text{Ca}_{1.90} \cdot \text{Al}_{9.25}\text{Si}_{10.75}\text{O}_{40.00} \cdot 10.96\text{H}_2\text{O}$	$I\ \bar{4}\ 2\ d$	17.3	NAT2005a01
tiptopite	$\text{K}_2\text{Li}_{2.9}\text{Na}_{1.7}\text{Ca}_{0.7} \cdot \text{Be}_6\text{P}_6\text{O}_{24} \cdot 2\text{OH}\ 1.3\text{H}_2\text{O}$	$P\ 6_3$	21.7	CAN1987a01
tschernichite	$\text{Ca}_4 \cdot \text{Al}_8\text{Si}_{24}\text{O}_{64} \cdot 32\text{H}_2\text{O}^1)$			BEA, [91Smi1, 93Bog1, 95Gal1]
vishnevite	$\text{Na}_8 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot \text{SO}_4\ 2\text{H}_2\text{O}$	$P\ 6_3$	16.6	CAN1984a01
wairakite	$\text{Ca}_7\text{Na} \cdot \text{Al}_{15}\text{Si}_{33}\text{O}_{96} \cdot 16\text{H}_2\text{O}$	$I\ 1\ 1\ 2/a$	19.0	ANA1979a01
willhendersonite	$\text{Ca}_2\text{K}_2 \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 10\text{H}_2\text{O}$	$P\ \bar{1}$	14.9	CHA1984c01
	$\text{Ca}_{2.9} \cdot \text{Al}_6\text{Si}_6\text{O}_{24} \cdot 11\text{H}_2\text{O}$	$P\ \bar{1}$	15.1	CHA1997a01

¹⁾ based on a tetragonal unit cell.

3 List of abbreviations

Just the abbreviations occurring in the text are listed. Further codes appearing in the Tables are explained in the corresponding chapters 8 to 15 of the introduction to volume B [2000Bau1].

a, b, c	Base vectors of the unit cell
<i>a, b, c, α, β, γ</i>	Unit cell constants [Å, °]
<i>B</i>	Isotropic displacement factor (temperature factor) [Å ²]
<i>B_{eq}</i>	Equivalent isotropic displacement factor [Å ²], calculated as explained in [88Fis1]
DLS	Distance Least Squares
DnR	Double ring consisting of two SnR's
e.s.d.	Estimated standard deviation
FD	Framework density defined as the number of tetrahedrally coordinated framework cations (T-atoms) per 1000 Å ³ [89Bru1].
FTC	Framework Type Code assigned by the SC-IZA.
<i>i</i>	<i>Klassengleiche</i> subgroups with identical space groups
IT	International Tables for Crystallography Vol. A [2002Hah1]
IZA	International Zeolite Association
<i>k</i>	<i>Klassengleiche</i> subgroups
n.p.d.	nonpositive definite

PU	Polyhedral Unit
SC-IZA	Structure Commission of the International Zeolite Association
SnR	Single ring containing n TX ₄ tetrahedra
t	<i>Translationengleiche</i> subgroups
T	Tetrahedrally coordinated framework cation
<i>x, y, z</i>	Fractional coordinates
X	Anion in the coordination sphere of the framework cation
<i>V</i>	Unit cell volume [Å ³]
ZSC	Zeolite Structure Code formerly assigned by the SC-IZA (replaced by FTC).

4 Polyhedral units, 1D-units, and 2D-nets

All units are described in the manner of [2000Smi1]. In addition we use the units listed in Table 4.1. For explanations see volume A and chapter 8 in volume B of this series.

Table 4.1 Additional PU's not listed in [2000Smi1].

<i>bb</i> unit	face symbol	point symmetry	occurrence
<i>bb01</i>	4 ⁴ 4 ⁴ 6 ⁴ 12 ²	2/ <i>m</i>	ATS
<i>bb02</i>	4 ² 4 ¹ 4 ¹ 4 ¹ 4 ¹ 6 ¹ 8 ² 10 ¹	<i>m</i>	AWO
<i>bb03</i>	4 ² 4 ¹ 4 ¹ 6 ² 10 ²	<i>m m</i> 2	BOG
<i>bb04</i>	4 ² 10 ²	<i>m m m</i>	BOG, CON, LAU
<i>bb05</i>	4 ² 4 ² 5 ² 5 ² 6 ² 8 ¹ 8 ¹ 8 ¹	<i>m</i>	BRE
<i>bb06</i>	4 ⁴ 4 ⁴ 4 ⁴ 6 ⁴ 8 ² 8 ²	2/ <i>m</i>	CGF
<i>bb07</i>	4 ⁴ 4 ⁴ 4 ⁴ 6 ⁴ 6 ⁴ 6 ⁴ 8 ² 10 ²	2/ <i>m</i>	CGF
<i>bb08</i>	4 ² 4 ² 4 ² 4 ¹ 8 ² 8 ¹ 10 ¹ 10 ¹	<i>m</i>	CGS
<i>bb09</i>	4 ² 6 ² 6 ¹	2	CHI
<i>bb10</i>	6 ² 6 ¹ 9 ² 12 ¹	2	CHI
<i>bb11</i>	5 ⁴ 12 ² 12 ²	2/ <i>m</i>	CON
<i>bb12</i>	6 ⁴ 6 ⁴ 14 ²	2/ <i>m</i>	CFI
<i>bb13</i>	4 ² 5 ⁴ 6 ² 12 ²	2/ <i>m</i>	BEA, CON
<i>bb14</i>	4 ² 6 ⁴ 6 ⁴ 8 ² 8 ²	2/ <i>m</i>	AEN
<i>bb15</i>	6 ² 8 ² 10 ²	<i>m m m</i>	DAC
<i>bb16</i>	5 ⁸ 6 ² 8 ² 10 ²	<i>m m m</i>	DAC
<i>bb17</i>	5 ⁴ 8 ² 10 ²	<i>m m m</i>	DAC, FER
<i>bb18</i>	4 ² 4 ¹ 5 ² 6 ² 6 ¹	<i>m m</i> 2	DON
<i>bb19</i>	6 ⁴ 6 ² 12 ²	<i>m m m</i>	GON, MTW
<i>bb20</i>	5 ⁴ 5 ⁴ 8 ² 10 ²	2/ <i>m</i>	HEU
<i>bb21</i>	4 ⁴ 4 ⁴ 5 ⁴ 5 ⁴ 8 ² 8 ²	2/ <i>m</i>	HEU
<i>bb22</i>	4 ⁴ 4 ² 5 ⁴ 6 ⁴ 6 ² 12 ²	2/ <i>m</i>	IFR
<i>bb23</i>	4 ² 12 ⁴	4/ <i>m m m</i>	ISV
<i>bb24</i>	4 ² 5 ² 6 ² 12 ¹	<i>m m</i> 2	ISV
<i>bb25</i>	4 ⁴ 4 ² 5 ⁴ 5 ⁴ 6 ⁴ 6 ⁴ 12 ⁴	<i>m m m</i>	ISV
<i>bb26</i>	4 ² 5 ⁴ 6 ⁴ 12 ²	<i>m m m</i>	ISV
<i>bb27</i>	4 ⁴ 4 ² 6 ⁴ 6 ² 6 ² 10 ²	2/ <i>m</i>	LAU
<i>bb28</i>	9 ⁴	$\bar{4}$ 2 <i>m</i>	LOV, RSN

Table 4.1 (continued)

<i>bb</i> unit	face symbol	point symmetry	occurrence
<i>bb29</i>	$3^2 4^1 8^1 9^2$	$m\ m\ 2$	LOV, NAB, RSN
<i>bb30</i>	$8^2 10^4$	$\bar{4}\ 2\ m$	MEL
<i>bb31</i>	$5^2 5^4 8^2 10^2$	$m\ m\ 2$	MFS
<i>bb32</i>	$4^2 5^4 5^6 8^2 8^2$	$2/m$	MTF
<i>bb33</i>	$6^2 6^2 10^2$	$m\ m\ 2$	MTT
<i>bb34</i>	$5^{12} 6^{12} 6^2 10^6$	$6/m\ m\ m$	MWW
<i>bb35</i>	$4^2 5^4 5^4 10^2$	$m\ m\ m$	MWW
<i>bb36</i>	$4^1 4^1 4^2 4^2 5^2 5^2 6^1 6^1 6^2 6^2 8^1 8^1$	m	RTE (type B)
<i>bb37</i>	$5^8 5^8 5^4 6^8 10^4$	$m\ m\ m$	NES
<i>bb38</i>	$3^4 3^4 3^4 3^4 8^4 8^4 14^2$	$2\ 2\ 2$	OSO
<i>bb39</i>	$4^2 4^2 6^2$	2	PON
<i>bb40</i>	$4^8 6^8 8^2$	$\bar{8}\ 2\ m$	RTE (type C)
<i>bb41</i>	$4^4 5^8 6^4 8^2$	$\bar{4}\ 2\ m$	RTE (type C)
<i>bb42</i>	$4^1 5^2 5^2 5^2 6^1 10^1 10^1$	m	MEL, MFI
<i>bb43</i>	$5^4 5^4 10^2$	$2/m$	MFI
<i>bb44</i>	$3^2 6^3$	$\bar{6}\ 2\ m$	NPO
<i>bb45</i>	$5^2 5^2 5^2 8^1 12^2$	$m\ m\ 2$	MOR
<i>bb46</i>	$5^4 6^4 12^2$	$m\ m\ m$	MTW
<i>bb47</i>	$3^4 3^4 3^4 4^1 8^4 8^1 10^4$	$4\ m\ m$	OBW
<i>bb48</i>	$5^2 5^2 6^4 8^2$	$2/m$	NSI
<i>bb49</i>	$4^2 4^1 4^1 8^2 8^2 8^2$	$m\ m\ 2$	OWE
<i>bb50</i>	$6^2 8^2$	$m\ m\ m$	OWE

5 Chemistry

In addition to the specifications given in chapter 10.2 of volume B [2000Bau1] the letter code R is introduced in the column for thermal treatment in Tables FTC.1.1 indicating rehydration of a dehydrated sample.

Table 5.1 List of sorbates and templates in entries of volumes B to D of this series.

code	description	chemical composition		occurrence
ABH	(±)-exo-2-aminobicyclo[2.2.1]heptane	$C_7H_{13}N$	$C_7H_{13}N$	RTE
1-Ada	1-adamantylamine	$C_{10}H_{17}N$	$C_{10}H_{17}N$	DDR, DOH, LEV
1-AdaOH	N,N,N-trimethyl-1-adamantylammonium hydroxide	$C_{10}H_{16}N(CH_3)_3OH$	$C_{13}H_{26}NO$	AFI
1-cb	1-chlorobutane	C_4H_9Cl	C_4H_9Cl	FAU
1-MI	1-methylimidazole	$C_3H_3N_2CH_3$	$C_4H_6N_2$	CHA

Table 5.1 (continued)

code	description	chemical composition		occurrence
1-propylamine	1-propylamine	$C_3H_7NH_2$	C_3H_9N	FER
1,2-dibromoethane	1,2-dibromoethane	$C_2H_4Br_2$	$C_2H_4Br_2$	LTA
1,6-dichlorohexane	1,6-dichlorohexane	$C_6H_{12}Cl_2$	$C_6H_{12}Cl_2$	MFI
18-crown-6	1,4,7,10,13,16-hexaoxacyclooctadecane	$C_{12}H_{24}O_6$	$C_{12}H_{24}O_6$	EMT, MSO
2-aminopentane	2-aminopentane	$CH_3CH(NH_2)C_3H_7$	$C_5H_{13}N$	NON
2-MCHA ⁺	protonated 2-methylcyclohexylammonium ⁺	$C_6H_{10}CH_3NH_3^+$	$C_7H_{16}N$	LEV
2-methylnaphthalene	2-methylnaphthalene	$C_{11}H_{10}$	$C_{11}H_{10}$	MFI
[2.2]cryptand	1,7,10,16-tetraoxa-4,13-diazacyclooctadecane	$C_{12}H_{28}N_2O_4^{2+}$	$C_{12}H_{28}N_2O_4$	MSO
[2.2.2]cryptand	hexacosa-4.7.13.16.21.24-diaza-1.10-bicyclo[8,8,8]hexacosane ²⁺	$C_{18}H_{38}N_2O_6^{2+}$	$C_{18}H_{38}N_2O_6$	LTA
acetone	Acetone	C_3H_6O	C_3H_6O	FAU
acetonitrile	acetonitrile	CH_3CN	C_2H_3N	LTA
acetylene	Acetylene	C_2H_2	C_2H_2	FAU, LTA
ammonia	Ammonia	NH_3	NH_3	FAU, LTA
aniline	aniline	C_6H_7N	C_6H_7N	FAU
BQ	benzylquinuclidinium ⁺	$C_{14}H_{20}N$	$C_{14}H_{20}N$	IFR
BQol	benzylhydroxyquinuclidinium ⁺	$C_{14}H_{19}(OH)N$	$C_{14}H_{20}NO$	IFR
benzene	benzene	C_6H_6	C_6H_6	FAU, LTL, MTW
BT	bithiophene	$C_8H_6S_2$	$C_8H_6S_2$	MFI
butadiene	butadiene	$CH_2CHCHCH_2$	C_4H_6	FAU
cHA	cyclohexylamine	$C_6H_{11}NH_2$	$C_6H_{13}N$	CHA
chloroform	chloroform	$CHCl_3$	$CHCl_3$	FAU
cyclohexane	cyclohexane	C_6H_{12}	C_6H_{12}	FAU
cyclopropane	cyclopropane	C_3H_6	C_3H_6	FAU, LTA
cyclotriazane	cyclotriazane	N_3H_3	N_3H_3	LTA
Co(DETA) ₂	Co-Bis(diethylenetriamine)	$Co((NH_2C_2H_4)_2NH)_2^{3+}$	$C_8H_{26}N_6Co$	CHA
Co(MCpD) ₂ F	Co-Bis(methylcyclopentadienyl) fluoride	$Co(C_5H_4CH_3)_2F$	$C_{12}H_{14}CoF$	DOH
(Cp) ₂ CoF	cobaltocenium fluoride	$CoF(C_5H_5)_2$	$C_{10}H_{10}CoF$	NON
(Cp) ₂ CoOH	bis(pentamethylcyclopentadienyl) cobalt(III) hydroxide	$CoF_{0.75}(OH)_{0.25}C_{20}H_{30}$	$C_{20}H_{30}CoF_{0.75}(OH)_{0.25}$	DON
DABCO	1,4-diazabicyclo[2,2,2]-octane (triethylenediamine)	$C_6H_{12}N_2$	$C_6H_{12}N_2$	AST, CGF
DDPOH	N,N-diethyl-3,5-dimethylpiperidinium hydroxide	$(C_2H_5)_2NC_5H_8(CH_3)_2OH$	$C_{11}NH_{25}O$	MEL
deutero benzene	deutero benzene	C_6D_6	C_6D_6	MFI
dibromobutane	dibromobutane	$C_4H_8Br_2$	$C_4H_8Br_2$	FAU
dichlorobenzene	dichlorobenzene	$C_6H_4Cl_2$	$C_6H_4Cl_2$	FAU
dinitrobenzene	dinitrobenzene	$C_6H_4(NO_2)_2$	$C_6H_4N_2O_4$	FAU
DiPDAP	N,N'-diisopropyl-1,3-diaminopropane	$(CH_3)_2CHNH_2(CH_2)_3NH_2CH(CH_3)_2^{2+}$	$C_9H_{24}N_2$	RHO

Table 5.1 (continued)

code	description	chemical composition		occurrence
DM	decamethonium ²⁺	$C_{16}H_{38}N_2^{2+}$	$C_{16}H_{38}N_2$	DFO
dodecane	dodecane	$CH_3(CH_2)_{10}CH_3$	$C_{12}H_{26}$	MFI
DPA	dipropylamine	$(C_3H_7)_2NH$	$C_6H_{15}N$	AEL, AFS, AFY, ATN, ATO, LTA
EAN	ethanolamine	$HO-CH_2CH_2-NH_2$	C_2H_7NO	APD, AWO
EDA	ethylenediamine (diaminoethane)	$H_2N-C_2H_4-NH_2$	$C_2H_8N_2$	ACO, AEN, AWO, FAU, FER, MER
EtOH	ethanol	C_2H_6O	C_2H_6O	FAU
ethylene	ethylene	C_2H_4	C_2H_4	FAU, LTA
ferrocene	ferrocene	$Fe(C_5H_5)_2$	$FeC_{10}H_{10}$	FAU
guanidinium	guanidinium	CH_6N_3	CH_6N_3	GIS
HCFC-124a	hydrochlorofluorocarbon-124a	CF_2HCF_2Cl	C_2HF_4Cl	FAU
hcha	protonated cyclohexylamine ⁺	$C_6H_{11}NH_3^+$	$C_6H_{14}N$	CHA
HDAB14	diprotated 1,4-diaminobutane	$C_4H_{14}N_2^{2+}$	$C_4H_{14}N_2$	OWE
HDAMP	diprotated 1,2-diamino-2-methylpropane	$C_4H_{14}N_2^{2+}$	$C_4H_{14}N_2$	EDI
HDAP12	diprotated 1,2-diaminopropane	$C_3H_{12}N_2^{2+}$	$C_3H_{12}N_2$	EDI
HDAP13	diprotated 1,3-diaminopropane	$C_3H_{12}N_2^{2+}$	$C_3H_{12}N_2$	EDI, GIS
HDMA	protonated dimethylamine ⁺	$(CH_3)_2NH_2^+$	C_2H_8N	GIS, HEU, RHO
HDPA	protonated dipropylamine ⁺	$(C_3H_7)_2NH_2^+$	$C_6H_{16}N$	GIS
HEDA	protonated ethylenediamine ⁺	$H_2N-C_2H_4-NH_3^+$	$C_2H_9N_2$	GIS
H ₂ EDA	diprotated ethylenediamine ²⁺	$H_3N^+-C_2H_4-NH_3^{2+}$	$C_2H_{10}N_2$	DFT, GIS, MFI
HETA	protonated diethylenetriamine ⁺	$C_4H_{14}N_3^+$	$C_4H_{14}N_3$	OWE
hexane	hexane	$CH_3(CH_2)_4CH_3$	C_6H_{14}	MFI, MTW
H ₂ DAH	diprotated diamino hexane ⁺	$H_3N^+-C_6H_{12}-NH_3^+$	$C_6H_{18}N_2$	KFI
HFC-134	hydrofluorocarbon-134	$HF_2C_2F_2H$	$C_2H_2F_4$	FAU
HiPA	protonated isopropylamine ⁺	$(CH_3)_2CHNH_3^+$	$C_3H_{10}N$	AFN, FAU
HMEA	protonated monoethylamine ⁺	$C_2H_5NH_3^+$	C_2H_8N	FAU, HEU
HMMA	protonated monomethylamine ⁺	$CH_3NH_3^+$	CH_6N	AEN, FAU, GIS, HEU, PON, RHO
HMMA(D)	deuterated monomethylamine ⁺	$CD_3ND_3^+$	CD_6N	RHO
HnPA	protonated n-propylamine	$C_3H_7NH_3^+$	$C_3H_{10}N$	HEU
H ₂ PMDA	diprotated pentamethylenediamine	$H_3N-C_5H_{10}-NH_3$	$C_5H_{16}N_2$	PHI
HPyr	protonated pyrrolidine	$C_4H_8NH_2^+$	$C_4H_{10}N$	GIS, NON
HPyridine	protonated pyridine ⁺	$C_5H_5NH^+$	C_5H_6N	LAU
hquin	protonated quinuclidine	$(C_2H_4)_3NHCH^+$	$C_7H_{14}N$	CGS, DDR
H ₃ tETA	triprotated triethylene tetramine	$C_6H_{21}N_4^{3+}$	$C_6H_{21}N_4$	GME
HTrMA	protonated trimethylamine	$(CH_3)_3NH^+$	$C_3H_{10}N$	RHO
HTrMA(D)	deuterated trimethylamine	$(CD_3)_3ND^+$	$C_3D_{10}N$	RHO
imidazole	imidazole ⁺	$C_3H_5N_2^+$	$C_3H_5N_2$	LAU
iPA	isopropylamine	$(CH_3)_2CHNH_2$	C_3H_9N	AWO, CHA, GIS

Table 5.1 (continued)

code	description	chemical composition		occurrence
MBA	methylbutylamine	$C_4H_9NHCH_3$	$C_5H_{13}N$	CHA
m-deb	m-dichlorobenzene	$C_6H_4Cl_2$	$C_6H_4Cl_2$	FAU
mesitylene	1,3,5-trimethyl-benzene	$C_6H_3(CH_3)_3$	C_9H_{12}	FAU
methanol	methanol	CH_3OH	CH_4O	LTA
methylene blue	methylene blue	$(H_3C)_2HNC_6H_3NS_C_6H_3N(CH_3)_2$	$C_{16}H_{16}N_3S$	FAU
methylene blue ⁺	methylene blue ⁺	$C_{16}H_{18}N_3S^+$	$C_{16}H_{18}N_3S$	MOR
methylpyrrole	methylpyrrole	C_5H_7N	C_5H_7N	FAU
MMA	monomethylamine	CH_3NH_2	CH_5N	PON
mor	morpholine ⁺	$(C_2H_4)_2ONH_2^+$	$C_4H_{10}NO$	CHA
MS	methyl sulfide	CH_3S	CH_3S	LTA
n-butene	n-butene	C_4H_8	C_4H_8	FAU
naphthalene	naphthalene	$C_{10}H_8$	$C_{10}H_8$	FAU, MFI
nitroaniline	nitroaniline	$NO_2C_6H_4NH_2$	$C_6H_6N_2O_2$	FAU, MFI, MTW
n-Mquin	N-methylquinuclidine	$(C_2H_4)_3NCHCH_3$	$C_8H_{16}N$	LEV
octane	octane	$CH_3(CH_2)_6CH_3$	C_8H_{18}	MFI
P3BZY	tripropylbenzylammonium ⁺	$(C_3H_7)_3NCH_2C_6H_5^+$	$C_{16}H_{28}N$	MFI
pdcB	p-dichlorobenzene	$C_6H_4Cl_2$	$C_6H_4Cl_2$	MFI
piperazine	piperazine	$C_4H_{12}N_2$	$C_4H_{12}N_2$	GIS
piperidine	piperidine	$C_5H_{10}NH$	$C_5H_{11}N$	DOH, ERI
PMDA	pentamethylenediamine	$H_2N-C_5H_{10}-NH_2$	$C_5H_{14}N_2$	CHA
Pyr	pyrrolidine	C_4H_8NH	C_4H_9N	AWO, MTN
pyridine	pyridine	C_5H_5N	C_5H_5N	CHA, FAU, FER, LTL, MFI, MTN
quin	quinuclidine	$(C_2H_4)_3NCH$	$C_7H_{13}N$	AST, AWW, DDR
quinF	quinuclidinium fluoride	$(C_2H_4)_3NHCHF$	$C_7H_{14}FN$	CLO
stilbene	stilbene	$C_{14}H_{12}$	$C_{14}H_{12}$	MFI
t-but	tert-butylamine	$C(CH_3)_3NH_2$	$C_4H_{11}N$	MTN
TCNQ	7,7,8,8-tetracyano-p-quinodimethane	$C_{12}H_4N_4$	$C_{12}H_4N_4$	FAU
tEA	triethylamine	$(C_2H_5)_3N$	$C_6H_{15}N$	AFI
TEA	tetraethylamine ⁺	$(C_2H_5)_4N^+$	$C_8H_{20}N$	AFT, CHA, LTA, MER, MTN
TEAOH	tetraethylamine hydroxide	$(C_2H_5)_4NOH$	$C_8H_{21}NO$	AEI
THF	tetrahydrofuran	$(CH_2)_4O$	C_4H_8O	MTN
thioindigo	thioindigo	$C_6H_4COSC_2SCOC_6H_4$	$C_{16}H_8O_2S_2$	FAU
thionin blue	thionin blue ⁺	$C_{12}H_{10}N_3S^+$	$C_{12}H_{10}N_3S$	MOR
TMA	tetramethylamine ⁺	$(CH_3)_4N^+$	$C_4H_{12}N$	CHA, EAB, FAU, GIS, MAZ, MTN
TMAF	Tetramethylamine fluoride	$(CH_3)_4NF$	$C_4H_{12}NF$	MTN
tMB	trimethylbenzene	C_9H_{12}	C_9H_{12}	FAU
TMAOH	tetramethylamine hydroxide	$(CH_3)_4NOH$	$C_4H_{13}NO$	ATT
TMPD	tetramethylpropanediamine	$C_3H_6(N(CH_3)_2)_2$	$C_7H_{18}N^2$	AWO

Table 5.1 (continued)

code	description	chemical composition		occurrence
toluene	methyl-benzene	$C_6H_5CH_3$	C_7H_8	FAU, MFI
TPA	tetrapropylammonium ⁺	$(C_3H_7)_4N^+$	$C_{12}H_{28}N$	MFI
TPAF	tetrapropylamine fluoride	$(C_3H_7)_4NF$	$C_{12}H_{28}FN$	AFI, MFI
TPAOH	tetrapropylamine hydroxide	$(C_3H_7)_4NOH$	$C_{12}H_{29}NO$	AFI, AFR, MFI
triazane	triazane	N_3H_5	N_3H_5	LTA
TrMA	trimethylamine	$(CH_3)_3N$	C_3H_9N	MTN, RHO
TTEAMBOH	1,3,5-tris(triethylammonium-methyl)benzenehydroxide	$C_6H_3(CH_2N(C_2H_5)_3)_3(OH)_3$	$C_{27}H_{57}N_3O_3$	BPH
TTF	tetrathiafulvalene	$C_6H_4S_4$	$C_6H_4S_4$	FAU
xylene	dimethyl-benzene	C_8H_{10}	C_8H_{10}	FAU, MFI

Fig. 5.1 shows the updated compilation of chemical elements occurring in all zeolites treated in volumes B, C and D. Tables 5.2 and 5.3 refer only to compounds covered in volume D.

		D																				He
H																				Ne		
Li	Be											B	C	N	O	F	Ar					
Na	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr					
K	Ca	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe					
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn					
Fr	Ra	A																				
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					

Fig. 5.1 Chemical elements (highlighted) occurring in all entries of volumes B to D with FTC's from ABW to RHO. Framework cations are in grey fields. Some of the framework atoms can also occur as exchangeable cations.

Table 5.2 Occurrence of framework cations in the crystal structures listed in volume D of this series.

	Li	Be	Mg	B	Al	Ga	Si	Ge	P	As	S	Ti	Cr	Mn	Fe	Co	Ni	Cu	Zn	Cd
LTA																				
LTL																				
LTN																				
MAR																				
MAZ																				
MEI																				
MEL																				
MEP																				
MER																				
MFI																				
MFS																				
MON																				
MOR																				
MOZ																				
MSO																				
MTF																				
MTN																				
MTT																				
MTW																				
MWW																				
NAB																				
NAT																				
NES																				
NON																				
NPO																				
NSI																				
OBW																				
OFF																				
OSI																				
OSO																				
OWE																				
PAR																				
PAU																				
PHI																				
PON																				
RHO																				

Table 5.3 Occurrence of nonframework cations in the crystal structures listed in volume D (FTC: LTA to RHO) of this series. The last column refers to the organic molecules and cations as listed in Table 5.1.

	H/D	Li	Na	K	Rb	Cs	Mg	Ca	Sr	Ba	Al	Tl	Mn	Fe	Co	Ni	Cu	Ag	Cd	NH ₄ org
LTA ¹⁾																				
LTL																				
LTN																				
MAR																				
MAZ																				
MEI																				
MEL																				
MEP																				
MER																				
MFI																				
MFS																				
MON																				
MOR ²⁾																				
MOZ																				
MSO																				
MTF																				
MTN																				
MTT																				
MTW																				
MWW																				
NAB																				
NAT																				
NES																				
NON																				
NPO																				
NSI																				
OBW																				
OFF																				
OSI																				
OSO																				
OWE																				
PAR																				
PAU																				
PHI																				
PON																				
RHO ²⁾																				

¹⁾ and: B, In, Pb, Zn, Eu²⁾ and: Pb

6 References

- 88Fis1 Fischer, R.X., Tillmanns, E.: *Acta Crystallogr. C* **44** (1988) 775.
- 89Bru1 Brunner, G.O., Meier, W.M.: *Nature* **337** (1989) 146.
- 91Smi1 Smith, J.V., Pluth, J.J., Boggs, R.C., Howard, D.G.: *J. Chem. Soc., Chem. Commun.* (1991) 363.
- 93Bog1 Boggs, R.C., Howard, D.G., Smith, J.V., Klein, G.L.: *Am. Mineral.* **78** (1993) 822.
- 95Gal1 Galli, E., Quartieri, S., Vezzalini, G., Alberti, A.: *Eur. J. Mineral.* **7** (1995) 1029.
- 2000Bau1 Baur, W.H., Fischer, R.X.: Zeolite-type crystal structures and their chemistry. Zeolite Structure Codes ABW to CZP. Subvolume B in Landolt-Börnstein, Numerical data and functional relationships in science and technology, New Series, Group IV: Physical Chemistry, Volume 14, Microporous and other framework materials with zeolite-type structures, Baur, W.H., Fischer, R.X. (eds.), Springer-Verlag, Berlin, 2000.
- 2000Smi1 Smith, J.V.: Tetrahedral frameworks of zeolites, clathrates and related materials. Subvolume A in Landolt-Börnstein, Numerical data and functional relationships in science and technology, New Series, Group IV: Physical Chemistry, Volume 14, Microporous and other framework materials with zeolite-type structures, Baur, W.H., Fischer, R.X. (eds.), Springer-Verlag, Berlin, 2000.
- 2002Bau1 Baur, W.H., Fischer, R.X.: Zeolite-type crystal structures and their chemistry. Framework Type Codes DAC to LOV. Subvolume C in Landolt-Börnstein, Numerical data and functional relationships in science and technology, New Series, Group IV: Physical Chemistry, Volume 14, Microporous and other framework materials with zeolite-type structures, Baur, W.H., Fischer, R.X. (eds.), Springer-Verlag, Berlin, 2002.
- 2002Hah1 Hahn, T.: *International Tables for Crystallography. Vol. A*, fifth revised ed., Kluwer Academic Publishers, Dordrecht, 2002.
- 2004Bau1 Baur, W.H., Fischer, R.X.: *Stud. Surf. Sci. Catal.* **154** (2004) 1254.
- 2004Fis1 Fischer, R.X., Baur, W.H.: *Stud. Surf. Sci. Catal.* **154** (2004) 1246.
- 2004Won1 Wondratschek, H., Müller, U.: *International Tables for Crystallography. Vol. A1*
- 2005ICS1 Inorganic Crystal Structure Database, Version 1.4.1, 2005-2, Fachinformationszentrum, Karlsruhe (2005).
- 2006Fis1 Fischer, R.X., Messner, T.: *STRUPLO 2006*, Univ. Bremen (2006).