8 Survey of NMR Parameters for Quadrupolar Nuclei in Powder Materials, in Particular for ^{27}Al, ^{23}Na and ^{17}O

Electric field gradient and chemical shift data for the three most commonly studied quadrupolar nuclei with half-integer spin, ^{27}Al, ^{23}Na, and ^{17}O, in inorganic powder materials are presented in Tables 8.1, 8.2 and 8.3, respectively.

The tables represent an incomplete collection of experimental data; calculated data are not included. Concerning the very usefull quantum chemical calculations, we refer to the review titled "Computing Electric Field Gradient Tensors" by Zwanziger [1]. He stated that "broadly speaking, outside the realm of systems dominated by dispersion forces, modern DFT (density functional theory) is accurate enough to provide a good description of the electronic structure and hence the EFG and quadrupole coupling in a very wide range of solids" [1].

For solid-state NMR studies of other quadrupolar nuclei in solid materials, we refer to the Web of Science Core Collection. A search in this data base returns for all quadrupolar nuclei the following numbers of publications from 1950 to the end of 2018:

deuterium-2	1488	calcium-43	77	rubidium-85	5	cesium-133	146
lithium-6	303	scandium-45	95	rubidium-87	86	barium-135	4
lithium-7	901	titanium-47/49	40	strontium-87	17	barium-137	10
beryllium-9	29	vanadium-50	1	zirconium-91	28	lanthanum-138	1
boron-10	4	vanadium-51	456	niobium-93	71	lanthanum-139	48
boron-11	305	chromium-53	4	molybdenum-95	59	hafnium-177	0
nitrogen-14	444	manganese-55	28	molybdenum-97	2	hafnium-179	0
oxygen-17	928	cobalt-59	80	technetium-99	19	tantalum-181	2
neon-21	0	nickel-61	4	ruthenium-99	8	rhenium-185/187	9
sodium-23	927	copper-63/65	102	ruthenium-101	1	osmium-189	1
magnesium-25	114	zinc-67	48	palladium-105	4	iridium-191	0
aluminum-27	4356	gallium-69/71	221	indium-113	9	iridium-193	0
sulphur-33	42	germanium-73	20	indium-115	33	gold-197	10
clorine-35/37	139	arsenic-75	24	antimony-121	16	mercury-201	4
potassium-39	61	bromine-79	37	antimony-123	5	bismuth-209	5
potassium-40	1	bromine-81	18	iodine-127	32		
potassium-41	0	krypton-83	2	xenon-131	8		

The search string *PY=1950-2018 AND (TS="NMR" OR TS="nuclear magnetic resonance") AND (TS="solid-state" OR TS="*MAS" OR TS="DOR")* was used for solid-state NMR, the extension *AND (TS= "H-2 NMR" OR TS= "2H NMR" OR TS= "deuterium NMR" OR TS= "solid-state H-2" OR TS= "H-2 MAS" OR TS= "deuterium-2")* was applied for ^{2}H NMR, and an extensions like *AND (TS= "aluminum-27" OR TS= "Al-27" OR TS= "27Al NMR")* were used for all other nuclei except boron-10 and boron-11, for which *"B-11 NMR"* was used instead of *"B-11"*. Combinations like *"Ti-47,49"* were added in some cases.

A very useful source of literature concerning special nuclei is the comprehensive and regularly updated compilation of quadrupole effects and their applications in solid-state NMR, presented by Pascal Man on his Internet page www.pascal-man.com.

Table 8.1. ^{27}Al, quadrupole coupling constant $C_\mathrm{Q} = e^2qQ/h$, the asymmetry parameter η, and the isotropic value of the chemical shift δ (referred to 1.0 M $AlCl_3\ 6H_2O$ [2]) for the ^{27}Al NMR of powder compounds at ambient temperature. The data published from 1983-1992 were compiled by Müller [3]. The acronym "qp" appears in the column for η, if the column C_Q contains the quadrupolar product parameter $P_\mathrm{Q} = C_\mathrm{Q}\sqrt{1+\frac{\eta^2}{3}}$ instead of C_Q.

Compound	site	C_Q/ MHz	η	δ /ppm	Refs.
Aluminum compounds without B, C, N, F, Si, P, S					
α-$Al(OH)_3$ (bayerite)	AlO_6	2.9	qp	11	[4]
	AlO_6-(1)	1.4	0.80	13.1	[5, 6]
	AlO_6-(2)	1.9	0.25	9.1	[5, 6]
γ-$Al(OH)_3$ (gibbsite)	AlO_6-(1)	2.2	qp	11	[7]
	AlO_6-Al(2)	2.2	0.75	10.5	[5]
	AlO_6-(2)	4.5	0.45	12	[7]
	AlO_6-Al(1)	4.7	1.00	17.2	[5]
	AlO_6-I	4.6	0.4	13.6	[6, 8]
	AlO_6-II	2.2	0.7	11.3	[6, 8]
α-AlO(OH) (diaspore)	AlO_6	3.4	0.8	17.0	[6, 9]
γ-AlO(OH) (boehmite)	AlO_6	-		9 (anisotr.)	[10]
	AlO_6	1.8-2.8	0.5-1.0	12.6	[5, 6]
α-Al_2O_3 (corundum)	AlO_6	2.40	0.01	18.8	[11]
α-Al_2O_3	AlO_6	1.58	qp	10.7	[12]
	AlO_6	2.38	0.0	13.5	[6, 13]
grain size 12-52 nm	AlO_6	2.4	0.05	16.0	[6, 14]
grain size 3.8 nm / 13 nm	AlO_4	2.4	-	71	[15]
	AlO_6	2.4	-	14	[15]
γ-Al_2O_3 (non-hydrated)	AlO_4	8.5	0.8	68	[16]
	AlO_6	5.5	0.7	13	[16]
γ-Al_2O_3 (hydrated)	AlO_4	5.1	-	71.5	[17]
	AlO_5	5.1	-	44.0	[17]
	AlO_6	3.55	-	10.0	[17]
grain size 3.8 nm / 13 nm	AlO_4	0.06	-	63	[15]
	AlO_5	0.06	-	43	[15]
	AlO_6	0.06	-	7	[15]
η- Al_2O_3 size 3.8 nm / 13 nm	AlO_6	0.08	-	−6	[15]
ρ-Al_2O_3	AlO_4, AlO_5, AlO_6	insufficiently resolved			[18]
κ-Al_2O_3	AlO_4	7.6	0.3	81.5	[19]
	AlO_6-(1)	5.0	-	ca. 13	[19]
	AlO_6-(4)	8.5	-	18	[19]
χ-Al_2O_3 (part. dehydr. gibbsite)	AlO_4	5.0	0.3	71.5	[20]
	AlO_5	2.7	0.3	38.5	[20]
	AlO_6	4.5	0.3	11.5	[20]
θ-Al_2O_3	AlO_4	6.4	0.65	80	[13]
	AlO_6	3.5	0	10.5	[13]
η-, γ-, δ-, θ-Al_2O_3	AlO_4	4.7-5.5	0.4-0.8	74-80	[21]
	AlO_6	3.0-4.0	0.4	11-15	[21]
CaO·6Al_2O_3	AlO_4	2.0	0_{assumed}	65	[22]
	AlO_5	6.7	0_{assumed}	27.5	[23]
	AlO_6-(1)	1.5	0_{assumed}	9	[22]
	AlO_6-(2)	<1	0_{assumed}	16	[22]
CaO·2Al_2O_3	AlO_4-(1)	6.7	0.8	78	[22]
	AlO_4-(2)	13	0.1	ca. 60	[22]

$CaO{\cdot}Al_2O_3$	AlO_4-(1)	2.7	0.85	80	[22]
	AlO_4-(2)	2.7	0.85	83	[22]
$4CaO{\cdot}3Al_2O_3$	AlO_4	2.4	0.95	80	[22]
$12CaO{\cdot}7Al_2O_3$	AlO_4-(1)	3.7	0.9	79	[22]
	AlO_4-(2)	11	0.2	85	[24]
$3CaO{\cdot}Al_2O_3$	AlO_4	9.7	0.3	85	[24]
	AlO_4-(1)	8.69	0.32	79.5	[25]
	AlO_4-(2)	9.3	0.54	78.25	[25]
$4CaO{\cdot}3Al_2O_3{\cdot}3H_2O$	AlO_4-(1)	1.8	0.5	78	[22]
	AlO_4-(2)	5.4	0.45	79	[22]
$CaAl_4O_7$	AlO_4-(1)	6.25	0.88	75.5	[26]
		6.4	0.90	68.1	[27]
	AlO_4-(2)	9.55	0.82	69.5	[26]
		9.5	0.82	59.1	[27]
$CaAl_{12}O_{19}$	site 1/2	3.2/4.2	0.0/0.0	65.7/20.0	[27]
	site 3/4/5	4.5/-/-	0.9/-/-	18.0/13.6/6.7	[27]
	site 1/2	0.15/21.4	-/0.00	16.25/55.8	[28]
	site 3/4/5	3.1/1.6/4.8	0.00/-/0.7	68.1/9.92/22.3	[28]
$SrAl_{12}O_{19}$	site 1/2	0.25/20.75	-/0.00	16.72/57.8	[28]
	site 3/4/5	3.45/1.35/4.9	0.00/-/0.65	67.5/9.45/22.1	[28]
	AlO_4/ AlO_4-d	3.455/20.71	0.5/0.00	67.90/56.91	[29]
	AlO_5	2.590	qp	19.50	[29]
	AlO_6-1/2	17.50/10.06	qp/qp	17.50/10.06	[29]
	AlO_6-3	4.990	0.65	21.73	[29]
$LaSrAl_3O_7$	site 1	3.0	0.5	75.4	[30]
	site 2	6.8	0.5	83.3	[30]
$LaSrAl_{1.5}Ga_{1.5}O_7$	site 1	4.2	0.5	78.7	[30]
	site 2	7.0	0.5	83.8	[30]
$CaAl_2O_4$	AlO_4-(1-5)	2.4-4.2	0.2-0.95	81.2-86.2	[26]
$Ca_{12}Al_{14}O_{33}$	AlO_4-(1)/(2)	9.7/3.8	0.4/0.7	85.9/80.2	[26]
$Ca_3Al_2O_6$	AlO_4-(1)/(2)	8.69/9.3	0.32/0.54	79.5/78.3	[26]
$CaAl_2H_{20}O_{14}$	AlO_6	2.4	qp	10.2	[26]
$Ca_3Al_2H_{12}O_{12}$	AlO_6	0.705	0.09	12.36	[26]
$Ca_4Al_2H_{26}O_{20}$	AlO_6	1.8	qp	10.2	[26]
$KAlO_2$	AlO_4	1.1	0.7	76	[24]
$KAlO_2{\cdot}0.5H_2O$	AlO_4	5.6	0.0	77	[24]
$KAlO_2{\cdot}H_2O$	AlO_4	6.5	0.6	83	[24]
$KAlO_2{\cdot}1.5H_2O$	AlO_4	5.0	0.25	81	[24]
$5BaO{\cdot}Al_2O_3$	AlO_4	2.3	0.8	80	[24]
$BaO{\cdot}Al_2O_3$	AlO_4	2.4	0.4	78	[24]
α-$BaO{\cdot}Al_2O_3{\cdot}2H_2O$	AlO_4-(1)/(2)	3.4/5.1	0.5/0.9	81/80	[24]
α-$LiAlO_2$	AlO_6	2.8	0.05	16	[31]
β-$LiAlO_2$	AlO_4	1.8	0.55	82	[31]
	AlO_4	1.86	0.56	83.0	[32]
γ-$LiAlO_2$	AlO4	3.2	0.7	81	[31]
single crystal	AlO_4	3.330	0.656	81.8	[33]
β-$NaAlO_2$	AlO_4	1.4	0.5	80	[24]
$NaAl_9O_{14}$	AlO_4	3.4	qp	55.9	[34]
	AlO_6	2.8	qp	9	[34]
$AlCl_3{\cdot}3Al(OH)_3{\cdot}6H_2O$	AlO_6	6.9	0.4	7	[3]
$AlCl_3{\cdot}4Al(OH)_3{\cdot}7H_2O$	AlO_6	5.7	0.7	3	[3]
$AlCl_3{\cdot}OPCl_3$	$AlCl_3O$	6.0	0.15	88	[35]
$Al_2Ge_2O_7$	AlO_5	8.8	0.4	36	[36]

$AlLaGe_2O_7$	AlO_5	7.2	0.37	36	[36]
$Al_2(MoO_4)_3$	AlO_6-(1)/(2)	1.12/0.88	0.65/0.95	−12.4/−13.4	[37]
	AlO_6-(3)/(4)	1.21/0.78	1.0/0.8	−10.3/−11.1	[37]
$MgAl_2O_4$ (spinel)	AlO_4	3.2	0.50	76.5	[38]
	AlO_6-1	3.73	0.26	14.5	[38]
	AlO_6-2	4.46	0.4	−1.0	[38]
$Cd_8(AlO_2)_{12}$ S_2 (sodalite)	AlO_4	2.00	< 0.1	80.4	[39]
$Ca_8(AlO_2)_{12}$ S_2 (sodalite)	AlO_4	3.55	< 0.1	79.1	[39]
$Cd_8(AlO_2)_{12}$ Se_2 (sodalite)	AlO_4	3.95	< 0.1	78.7	[39]
$Cd_8(AlO_2)_{12}$ $(SO_4)_2$ (sodalite)	AlO_4	3.24	< 0.1	79.1	[39]
$Sr_8(AlO_2)_{12}$ S_2 (sodalite)	AlO_4	4.65	< 0.1	76.9	[39]
$Sr_8(AlO_2)_{12}$ Se_2 (sodalite)	AlO_4	5.10	< 0.1	76.6	[39]
$Sr_8(AlO_2)_{12}$ $(CrO_4)_2$ (sodalite)	AlO_4	6.75	< 0.1	75.5	[39]
$SrAl_{12}O_{19}$	AlO_4	3.45	0.1	68.0	[40]
	AlO_5	2.1	0.7	18.0	[40]
	AlO_6-(1)	0.6	1	17.1	[40]
	AlO_6-(2)	1.3	1	9.6	[40]
	AlO_6-(3)	4.9	0.63	21.7	[40]
$Sr_4Al_{14}O_{25}$	Al1/Al2/Al3	4.4/5.2/4.2	0.8/0.8/0.2	78/82/77	[41]
	Al4/Al5/Al5	2.4/6.8/9.2	0.1/0.2/0.0	12/12/11	[41]
$YAlO_3$	AlO_6	1.61	qp	10.7	[12]
$Y_4Al_2O_9$	AlO_4-1	10.81	0.48	78.2	[12]
	AlO_4-2	10.36	0.77	76.2	[12]
$Y_3Al_5O_{12}$	AlO_6	1.13	qp	2.1	[12]
	AlO_4	6.21	0.05	77.5	[12]
	AlO_6	1.13	qp	2.1	[12]
$Y_3Al_5O_{12}$ (YAG II 800)	AlO_6/AlO_5	-	-	1.2/23.6	[42]
	AlO_4	6.0	0.08	76.6	[42]
$Y_3Al_5O_{12}$ (YAG)	AlO_6	0.6	-	5.38	[43]
	AlO_4	6.1	-	82	[43]
$AlVO_4$	Al1	1.64	0.30	−8.9	[44]
	Al2	6.73	0.42	27.2	[44]
	Al3	5.88	0.58	−1.1	[44]
ZrO_2-Al_2O_3 (co-hydrolysis,	AlO_4/ AlO_5	10.0/5.0	-	78/37	[45]
annealed at 1000 °C)	AlO_6	7.0	-	16	[45]
MgO-Al_2O_3 (annealed at 600 °C)	AlO_4	10.5	-	82	[45]
	AlO_5	10.0	-	41	[45]
	AlO_6	7.0/2.0	-	17/15	[45]
Na_3AlH_6 doped/non-doped		0.52/0.70	0.5/0.2	−42.7/−42.5	[46]
Na_2LiAlH_6		<0.1	-	−46	[46]
$NaAlH_4$		3.15	0.04	97.5	[46]
ZrNiAl	Al-Ni	3.3	0.42	393	[47]

Aluminosilicates

$Al_2Si_2O_5(OH)_4$ (kaolinite)	AlO_6	3.6	qp	7	[7]
	AlO_6 (1)/(2)	3.4/3.0	0.8/0.9	7.5/8.0	[48]
Al_2SiO_5 (sillimanite)	AlO_4	6.77	0.53	64.5	[49]
	AlO_4	6.74	0.51	63.9	[50]
	AlO_6	8.93	0.46	4.0	[49]
	AlO_6	8.83	0.49	4.7	[50]
Al_2SiO_5 (andalusite)	AlO_5	5.6	0.76	35.2	[51]
	AlO_6	15.3	0.13	11.9	[51]
Al_2SiO_5 (kyanite)	AlO_6-(1)/(2)	10.1/3.8	0.27/0.85	13.0/4.0	[51]
	AlO_6-(3)/(4)	6.4/9.2	0.70/0.38	5.7/5.9	[51]
$Al_4Si_8O_{20}(OH)_4$ (pyrophillite)	AlO_6			4.3	[52]
dehydroxylate (550 °C)	AlO_5	10.5	0.6	29	[52]
$K_{1.5}Al_4(Si_{6.5}Al_{1.5})O_{20}(OH)_4$ (illite)	AlO_4	2.9	-	72.4	[53]
	AlO_6	3.7	-	6.0	[53]
$3Al_2O_3{\cdot}SiO_2$ (mullite)	AlO_6	7.3	0	6.3	[54]
	AlO_4 (T)/(T')	7.3/6	0/0.5	68/53	[54]
	AlO_4 (T*)	4	0.5	45	[54]
$2Al_2O_3{\cdot}SiO_2$ (2:1 mullite)	AlO_6 site 1	4.5	qp	7.5	[55]
	site 2	3.2	qp	49	[55]
	AlO_4 site 3	4.6	qp	69.4	[55]
$3Al_2O_3{\cdot}2SiO_2$ (mullite precursor	site 1a/1b	4.3/3.4	qp/qp	7/15	[56]
obtained by sol-gel synthesis)	site 2	4.3	qp	37	[56]
	site 3	4.1	qp	71	[56]
$Mg_3Al_2Si_3O_{12}$ (pyrope)		1.0	0.5	2.9	[57]
$Ca_3Al_2Si_3O_{12}$ (grossular)		3.7	0.2	−3.35	[57]
$Ca_2Al_3Si_3O_{12}$-(OH) (zoisite)	AlO_6 1/2	7.9/18.4	0.51/0.16	10.7/8.0	[58]
	AlO_6 1/2	8.0/18.19	0.53/0.13	10.7/7	[59]
$CaAlAlSiO_6$ (clinopyroxene)	AlO_6 a/b/c	5.0/4.6/5.6	0.5/0.7/0.7	2.7/8.6/13.5	[60]
	AlO_4 d/e	5.4/11.8	0.5/0.45	66.5/79.7	[60]
$Sr_3Al_{10}SiO_{20}$	Al(1)/ Al(2)	3.73/8.13	0/0.3	7.2/12.0	[61]
	T_2(4Al)	2.61	0	82.0	[61]
	T_1+T_2(*n*Al, *m*Si)	6.86	0.3	78.0	[61]
$(Mg,Fe,Al)_6(Si,Al)_4O_{11}(OH)_8$	AlO_4	2.8	-	72	[49]
(pennine, penninite)	AlO_6	1.4	-	10	[49]
$KAlSi_2O_6$ (leucite)	T1/T2/T3	2.07/2.58/2.34	qp	61.0/63.9/69.2	[62]
$CaAl_2Si_2O_8$ (anorthite)	6 sites	2.7—8.2	0.45-0.70	61-66	[62]
$Na_{16}Ca_{16}(AlO_2)_{48}(SiO_2)_{72}$ (mesolite)	Al(1)	3.0	0	64.4	[63]
	Al(2)/ Al(3)	1.9/2.0	0/0	62.6/65.1	[63]
$KAl_2[(OH,F)_2/AlSi_3O_{10}]$	AlO_4	2.1	-	72	[49]
(muscovite)	AlO_6	2.2	-	5	[49]
$CaAl_2[(OH)_2/Al_2Si_2O_{10}]$	AlO_4	4.2	-	76	[49]
(margarite)	AlO_6	6.3	-	11	[49]
$CaMg_3Al_2Si_2O_{10}(OH)_2$	AlO_4	2.8	-	76	[49]
(xantophyllite)	AlO_6	2.0	-	11	[49]
$Na_8Al_2Be_2Si_8O_{24}Cl_2$ (tugtupite)	AlO_4	1.36	0.08	63.4	[64]
$NaAlSi_3O_8$ (low albite)	AlO_4	3.29	0.62	62.7	[65]
$Na_2Al_2Si_3O_{10}{\cdot}2H_2O$ (natrolite)	AlO_4	1.67	0.50	64	[49]
$Na_2Al_2Si_3O_{10}{\cdot}2H_2O$ (tetranatrolite)	AlO_4 T1/T2	2.2/2.4	qp/qp	63.1/64.2	[66]
$KAlSi_3O_8$ (microcline)	AlO_4	3.22	0.21	58.5	[65]
Na,K $AlSi_3O_8$ (feldspar)	8 samples	3.15-4.0	0.25-0.52	59.2-61.0	[67]
(Mg, Fe)Al_3SiBO_9 (grandidierite)	AlO_5	8.7	0.95	41.0	[68]
	AlO_6-(1)/(2)	3.5/8.6	0.5/0.95	9.0/11.0	[68]

$NaCa_2Mg_4Al(Si_6Al_2)O_{22}(OH)_2$ (pargasite)	AlO_4 (Q^3)	4.0	qp	77	[69]
$NaCa_2Mg_5Al(Si_7Al)O_{22}F_2$	AlO_4 (Q^2)	3.0	qp	76	[69]
(fluor edenite)	AlO_4 (Q^3)	5.9	qp	77	[69]
$Na_8Cl_2[Al_6Si_6O_{24}]$ (NaCl-sodalite)		0.7	qp	64.7	[70]
$Na_8Cl_2[Al_6Si_6O_{24}]$ (blue sodalite)	AlO_4	1.45	0.1	40	[71]
$Na_{8.0}Cl_{1.8}[AlSiO_4]_6 \cdot 0.4\ H_20$	AlO_4	0.94	0.32	62.9	[72]
$Na_8Br_2[Al_6Si_6O_{24}]$ (NaBr-sodalite)		0.8	qp	63.2	[70]
$Na_8I_2[Al_6Si_6O_{24}]$ (NaI-sodalite)		0.6	qp	61.2	[70]
$Na_8[Al_6Si_6O_{24}]\cdot(H_3O_2)_2$ (basic sodalite)		0.8	qp	64.5	[73]
$Na_8Br_2\ [Al_6Si_6O_{24}]\ \cdot$ (basic sodalite)		0.8	qp	63.4	[73]
$Na_{7.7}Br_{1.8}[AlSiO_4]_6 \cdot 0.4\ H_20$	AlO_4	0.81	0.29	61.8	[72]
$Na_6[Al_6Si_6O_{24}]\cdot(4H_2O)_2$ (hydro sodalite)		2.2	qp	65.6	[73]
$Na_8Br_2\ [Al_6Si_6O_{24}]$ (dry sodalite)		0.8	qp	63.4	[73]
$Li_{7.6}Na_{0.4}Cl_{1.9}[AlSiO_4]_6 \cdot 0.7\ H_20$	AlO_4	0.98	0.59	71.9	[72]
$Li_{7.3}Na_{0.3}Br_{1.8}[AlSiO_4]_6 \cdot 1.1\ H_20$	AlO_4	0.71	0.61	70.9	[72]
$Na_{7.8}I_{1.7}[AlSiO_4]_6 \cdot 0.6\ H_20$	AlO_4	0.57	0.34	60.4	[72]
$Ca_8(OH)_8Al_8Si_4O_{24}$ (sodalite)	AlO_4	5.3	0.24	-	[74]
$Na_6\ [AlSiO_4]_6$ (sodalite)		2.7	$0_{assumed}$	54	[75]
$Na_6Zn_2[AlSiO_4]_6(SO_4)_2$ (sodalite)		2.5	$0_{assumed}$	58	[75]
Zeolite Na-A (hydrated)	AlO_4	1.1	0.75	59.2	[49]
Zeolite H, Na-A (dehydrated)	AlO_3	12	-	-	[76]
Zeolite Na-Y (hydrated)	AlO_4	2.0	0.5	62.8	[49]
Zeolite Na-Y (dehydrated)	AlO_4	5.5	0.3	ca. 60	[77]
Zeolite H-Y (dehydrated)	AlO_3	13.1	0.75	105±20	[77]
	AlO_3	15.3	0.4	60	[78]
Zeolite Al, Na-Y (dehydrated)	AlO_4/Al^{x+}	14.5	0.3	70	[16]
	AlO_4/Na^+	5.5	0.8	60	[16]
	Al^{x+}cat.	6.0	0.7	35	[16]
Zeolite H, Na-Y (hydrated)	AlO_4/H^+	16.0/14.0	0.3	70	[16]
	AlO_4/Na^+	5.5	0.8	60	[16]
Dealumin. H, Na-Y (hydr.)	AlO_4/H^+	15.0	0.3	70	[16]
	AlO_4/Na^+	8.0	0.8	65	[16]
	Al^{x+}cat.	7.5	0.7	35	[16]
	AlO_6 cluster	5.0	0.7	10	[16]
Zeolite USY (hydrated)	AlO_4/ AlO_5/ AlO_6	2.8/4.1/2.9	-	60.0/34.5/4.0	[17]
	AlO_4 (4 sampl.)	1.9-7.5	qp	60.5-69.7	[79]
	AlO_5 (4 sampl.)	3.9-4.6	qp	34.0-39.8	[79]
	AlO_6 (4 sampl.)	1.9-3.2	qp	0.1-7.5	[79]
Zeolite Ti-USY	AlO_4	2.0/1.5	qp/qp	64.4/61.1	[80]
	AlO_5	3.2	qp	33.9	[80]
	AlO_6	2.0/1.6	qp/qp	6.0/0.01	[80]
Zeolite H-MOR (dehydrated)	AlO_3	15.0	0.35	-	[81]
	AlO_4	6.8	0.7	-	[81]
Zeolite NH_3(H)-MOR	$AlO_4(NH_4)$/(H)	1.9/5.6	qp/ qp	45/35	[82]
Zeolite BEA (Si/Al=9-215)	Td1	2.3-2.5	qp	57.5-59.0	[83]
	Td2	1.7-1.9	qp	53.5-54.0	[83]
Zeolite H-BEA (Si/Al=9-215)	Td1	1.0-2.0	qp	58.5-60.0	[83]
	Td2	1.1-1.7	qp	55.0-60.0	[83]
Zeolite H-BEA (dehydrated)	AlO_3	16	0.1	-	[76]
Zeolite BEA (3 samples)	AlO_4 (2b)	2.3-2.4	qp	58.0-58.4	[84]
	AlO_4 (2a)	1.5-1.8	qp	53.9-54.2	[84]
	AlO_6	-	-	≈0	[84]

Zeolite Na-ZSM-5 (dehydrated)	AlO_4	4.7	0.5	≈60	[77]
Zeolite H-ZSM-5 (dehydrated)	AlO_3	16.0	0.1	82±20	[77]
	AlO_3	15.5	0.5	-	[81]
	AlO_4	7.3	0.7	-	[81]
Zeolite ZSM-5 Si/Al=14-250, 7 samples					
	AlO_4, Peak I	1.6-1.7	qp	54.4-55.7	[85]
	AlO_4, Peak II	1.5-1.6	qp	52.2-52.3	[85]
Zeolite TPA-ZSM-5	AlO_4 (1)/(2)	1.4/1.8	qp/ qp	52.2/54.9	[86]
Zeolite H-ZSM-5	AlO_4(1)/(2)	1.2/1.6	qp/ qp	55.5/56.5	[86]
Zeolite NH_3(H)-ZSM-5	AlO_4(1)/(2)	1.2/1.6	qp/ qp	53.8/56.4	[86]
Zeolite TNU-9	AlO_4	2.1-2.3	qp	53.5-57.2	[87]
Zeolite Li-CHA (hydrated)	AlO_4	2.4	qp	60.0	[88]
Zeolite Li-CHA (dehydrated)-I	AlO_4	5.3	qp	62	[88]
Zeolite Li-CHA (dehydrated)-II	AlO_4	7.3	qp	57	[88]
Zeolite Na-CHA (hydrated)	AlO_4	1.8	qp	59.5	[88]
Zeolite Na-CHA (dehydrated)	AlO_4	4.2	qp	61	[88]
Zeolite K-CHA (hydrated)	AlO_4	1.8	qp	59.5	[88]
Zeolite K-CHA (dehydrated)	AlO_4	2.9	qp	60	[88]
Zeolite ITQ-33	T4	1.11/1.12	qp	52.38/53.46	[89]
	T3	2.20/2.21/2.19	qp	60.75/62.07/63.22	[89]
H, Al-MCM-41 (as synthesized)	AlO_4	2.3	$0_{assumed}$	52.6	[90]
Al_2O_3-B_2O_3-SiO_2-Na_2O glasses		3.7-4.2	qp	59-63	[91]
$0.5Al_2O_3$–$xSiO_2$ glasses	AlO_4	5.3-6.5	qp	59-68	[92]
with $1 \leq x \leq 6$	AlO_5	4.6-5.3	qp	32-37	[92]
	AlO_6	3.9-4.6	qp	3-6	[92]
Na_2O-CaO-Al_2O_3-SiO_2 glass ANCS	AlO_4	6.8	-	60.5	[93]
	AlO_5	7.4	-	34.7	[93]

Phosphorous containing materials

$AlPO_4$ (quartz)	AlO_4	4.2	0.35	44.8	[94]
$AlPO_4$ (tridimite)	AlO_4	0.75	0.95	39.8	[94]
$AlPO_4$ (cristobalite)	AlO_4	1.2	0.75	42.5	[94]
$Al_2PO_4(OH)_3$ (augelite)	AlO_5/ AlO_6	5.5/4.7	0.78/0.2	30/–3	[95]
$Al_2PO_4(OH)_3{\cdot}H_2O$ (senegalite)	AlO_5	2.87	$0_{assumed}$	30	[95]
	AlO_6	4.09	$0_{assumed}$	1.7	[95]
$KAlP_2O_7$	AlO_6	1.2	0.25	–16	[96]
$Zn_3Al_6(PO_4)_{12}$	site 1/ site 2	1.6/1.23	0.4/0.6	49.74/47.6	[97]
$AlPO_4$-5 (hydrated)	AlO_4	2.3	0.95	40.4	[94]
$AlPO_4$-8 (dehydrated)	AlO_4-(1)/(2)	3.9/3.6	$0.5_{ass.}$/ $0.5_{ass.}$	40.1/40.6	[98]
	AlO_4-(3)/(4)	3.6/3.0	$0.5_{ass.}$/ $0.5_{ass.}$	47.0/42.9	[98]
	AlO_4-(5)	3.4	$0.5_{assumed}$	42.6	[98]
$AlPO_4$-14 (hydrated)	AlO_5-(Al1[99])	5.66	0.89	27.2	[100]
	AlO_5-(3)(Al1[99])	5.58	0.97	27.1	[101]
	AlO_5-Al1	5.6	1.0	27	[102]
	AlO_4-(Al2 [99])	4.15	0.82	44.0	[100]
	AlO_4-(2)(Al2 [99])	4.08	0.82	43.5	[101]
	AlO_4-Al2	4.1	0.8	44	[102]
	AlO_4-(Al3 [99])	1.75	0.70	43.2	[100]
	AlO_4-(1)(Al3 [99])	1.74	0.63	42.9	[101]
	AlO_4-Al3	1.7	0.6	43	[102]
	AlO_6-(Al4 [99])	2.60	0.68	–0.9	[100]
	AlO_6-(5)(Al4 [99])	2.57	0.7	–1.3	[101]
	AlO_4-Al4	2.6	0.7	–1	[102]

$AlPO_4$-14 (dehydrated)	AlO_4-Al1	4.0	0.8	43	[102]
	AlO_4-Al2	3.4	0.2	43	[102]
	AlO_4-Al3	2.5	0.6	38	[102]
	AlO_4-Al4	4.9	0.3	45	[102]
$AlPO_4$-14A (dehydrated)	AlO_4-Al1	4.5	-	63.4	[103]
	AlO_4-Al2	4.1	-	43.1	[103]
	AlO_4-Al3	4.7	-	45.5	[103]
	AlO_4-Al4	2.6	-	–14.9	[103]
$AlPO_4$-15	Al1	3.1	0.8	2.5	[104]
	Al2	3.1	0.8	–5.0	[104]
$AlPO_4$-21 (hydrated)	AlO_4	8.3	0.15	47.3	[105]
	AlO_5-(1)/(2)	5.9/7.4	0.68/0.52	14.6/15.7	[105]
$AlPO_4$-25 (hydrated)	AlO_4-(1)/(2)	1.9/0.8	$0.67_{ass.}/0.67_{ass.}$	40.8/39.5	[105]
$AlPO_4$-25 (dehydrated)	AlO_4-(1)	2.3/1.1	$0.67_{ass.}/0.67_{ass.}$	39.2/37.5	[105]
$AlPO_4$-34 (six samples)	$Al1_{octa}$	1.3-2.2	qp	–5.1-–4.0	[106]
	$Al2_{tetra}$	2.0-2.9	qp	42.7-46.7	[106]
	$Al3_{zetra}$	2.5-4.4	qp	46.0-48.0	[106]
$AlPO_4$-53 (hydr. and dehydr.)	sites Al1-Al6	2.0-9.2	0-0.9	17-45	[107]
$AlPO_4$-ZON	site Al1	3.8	qp	50.6	[108]
	site Al2	3.6	qp	43.0	[108]
	site Al3	4.9	qp	27.2	[108]
	site Al4	6.3	qp	24	[108]
$AlPO_4$-SOD as-synthesized	Al1/2/3	2.3/2.4/2.7	0.79/0.79/0.82	38/41/–8.5	[92]
dehydrated at 200 °C	Al1/2/3	2.6/2.8/2.6	0.99/0.42/0.92	39/37/36	[92]
	Al4/5	2.7/2.4	0.35/0.98	12/–12	[92]
$AlPO_4$-STA-2	Al1/Al2	2.0/3.5	0.7/0.9	36.0/42.0	[109]
	AlO_4 3 sites	2.4/3.6/2.1	qp/qp/qp	39/45/49	[110]
	AlO_5	3.1	qp	17	[110]
Layered aluminophosphates	6 sites	1,3-5.8	0.1-1.0	–17.6-48.1	[111]
$x Al_2O_3\cdot (30-x)P_2O_5\cdot 70SiO_2$	AlO_4	4.0-6.3	qp	40.1-61.5	[112]
x=2.5-27.5% (glass)	AlO_5	4.0-6.0	qp	9.4-35.0	[112]
	AlO_6	4.0-5.0	qp	–20.4-5.0	[112]
$AlPW_{12}O_{40}$ dehydrated at 473 K	AlO_6	2.4/6.0	1/0.8	2/4	[113]
	AlO_5	7.0/8.7	0.2/0.2	24/44	[113]
	AlO_4	8.5	0.8	65	[113]
60 $NaPO_3$ 40AlF_3 glass	$Al^{(6)}$/ $Al^{(5)}$/ $Al^{(4)}$	5.1/6.0/3.3	-	–4.5/19/44	[114]

Boron containing materials

AlB_2		0.533	-	880	[115]
$2SrO\cdot Al_2O_3\cdot B_2O_3$	AlO_4	4.3	0.65	83.5	[116]
$2CaO\cdot Al_2O_3\cdot B_2O_3$	AlO_4	6.25	0.45	79.5	[116]
$2Li_2O\cdot Al_2O_3\cdot B_2O_3$	AlO_4	6.0	0.45	76	[116]
$3Li_2O\cdot Al_2O_3\cdot 2B_2O_3$	AlO_4	6.7	0.83	70	[116]
$9Al_2O_3\cdot 2B_2O_3$	AlO_4	6.8	0.1	53	[116]
	AlO_5	4.8	0.3	31	[116]
	AlO_6	6.2	0.4	10.5	[116]
$Al_{6-x}B_xO_9$ (mullite structure)	$AlO_{4\ or\ 5}$	3.9-9.0	-	33.0-67.8	[117]
8 samples with $1 \leq x \leq 4$	AlO_6	4.0-10.5	-	5.1-21.9	[117]
$Na_2Al_2B_2O$	AlO_4	1.65	0.05	70.3	[118]
$Li_6Al_2(BO_3)_4$		6.4	0.88	69.3	[119]

Flour containing materials

AlF_6^{3-} octahedrons, fluoroaluminates		0.065-1.58	0-0.95	–7-1	[120, 121]
AlF_3		0.213	0.0	-	[122]
α-AlF_3	AlF_6	2.8	0	–13.2	[123]
β-AlF_3	AlF_6	3.4	0	–12.5	[123]
β-$AlF_{6-x}(OH)_x$ (82 m^2 g^{-1})	AlF_6 and $AlF_5(OH)$	0.28	qp	–15.5	[124]
	$AlF_4(OH)_2$	0.61	qp	–11.7	[124]
	$AlF_3(OH)_3$	0.990	qp	–9.5	[124]
HS-AlF_3	site A/B	3.88/8.68	qp/qp	4.8/–7.9	[125]
	site C/D	6.37/5.04	qp/qp	–7.4/–7.7	[125]
$H_3AlF_6{\cdot}6H_2O$	AlF_6	0.3	0.0	–2.8	[126]
$K_2AlF_5{\cdot}H_2O$	AlF_6	12	0.0	0	[126]
$RbAlO_2$	5 sites	2.7-8.7	0.03-0.65	20.5-69.9	[127]
$Rb_2Al_2O_2F_2$	AlO_4	9.7	0.00	67.8	[127]
$RbAlF_4$	AlF_6	13	0.1	–4	[126]
$Rb_2AlF_5{\cdot}H_2O$	AlF_6	13	0.0	0	[126]
$CsAlF_5{\cdot}H_2O$	AlF_6	7.5	0.15	–10	[126]
NH_4AlF_4	AlF_6	10	0.1	–6	[126]
$KAlF_4$	AlF_6	12	0.0	–5	[126]
	AlF_6	-	-	–19.5	[128]
K_3AlF_6	AlF_6	-	-	–1.2	[128]
Tl_2AlF_5	AlF_6	-	-	–0.8	[128]
α-$BaAlF_5$	AlF_6	-	-	–13.4	[128]
β-Ba_3AlF_9	3 sites	0.14-0.51	0.07-0.85	–2-1	[129]
$Ba_3Al_2F_{12}$	AlF_6	-	-	–11.7	[128]
β-$CaAlF_5$		1.53	0.10	-	[130]
$Al_{13}Si_5O_{20}(OH,F)_{18}Cl$ (zunyite)	$Al1_{Keggin}$	2.25	1.0	72.2	[131]
	$Al1_{Pentamer}$	1.96	0.7	46.5	[131]
	$Al2_{without\ F}$	2.80	0.4	7.8	[131]
	$Al2_{with\ one\ F}$	7.08	0.4	14.0	[131]
$Al_2SiO_4F_2$ (topas)	AlF_6	1.7	0.4	0.3	[126]
Na_3AlF_6 (cryolite)	AlF_6	0.58	0.89	–0.5	[132]
	AlF_6	0.600	0.9	-	[122]
	AlF_6			–0.8	[128]
	AlF_6	2.0	0	1.4	[123]
K_2NaAlF_6 (elpasolite)	AlF_6	1.4	0	0.8	[123]
$Na_5Al_3F_{14}$	AlF_6 1/2	8.2/6.5	0/1	–1/–3	[123]
Na_2MgAlF_7 (weberite)	AlF_6	2.15	0.56	–5.4	[132]
$Na_3Al_2Li_3F_{12}$ (cryolithionite)	AlF_6	1.03	0.09	–0.5	[132]
$Na_5Al_3F_{14}$ (chiolite)	AlF_6	8.0	0.13	–2.5	[132]
	AlF_6 1/2	5.867/8.000	0.0/0.1	-	[122]
$Na_2Ca_3Al_2F_{14}$	AlF_6	0.433	0	–1.6	[133]
α-$NaCaAlF_6$	AlF_6 (i)/(ii)	3.800/2.933	0.25/0.1	–3.4/–2.2	[133]
β-$NaCaAlF_6$	AlF_6 (i)/ (ii)	1.300/0.400	0/0	–3/–3	[133]
60 $NaPO_3$ 40AlF_3 glass	$Al^{(6)}$/ $Al^{(5)}$/ $Al^{(4)}$	5.1/6.0/3.3	-	–4.5/19/44	[114]

Nitrogen containing materials

$AlO_{4-x}N_x$ (AlON) and $(Si, Al)_x(O, N)_{x+1}$ (SiAlON) materials, see [134], for ceramic [135]

SiAlON	AlO_6	-		2.8	[136]
γ-AlON	AlO_6	-	-	14	[137]
SiAlON	AlO_4	-		59	[136]
γ-AlON	AlO_4	-	-	66	[137]
AlON or Al_2O_3/AlN composite	$AlNO_3$	-	-	96	[137]
AlON or Al_2O_3/AlN composite	AlN_2O_2	-	-	96	[137]
AlON or Al_2O_3/AlN composite	AlN_3O	-	-	106	[137]
AlN	AlN_4	-	-	114-117	[137]
$CaMg_2AlN_3$	AlN_4	5.6	-	120	[138]

Other aluminum compounds

Al_4C_3	Al1	15.58	0	120.1	[139]
	Al2	15.83	0	111.2	[139]
$Al(acac)_3$	AlO_6	3.03	0.15	0.0	[140]
$Al(trop)_3$		4.43	0.08	36.6	[140]
$Al(TMHD)_3$	AlO_6	3.23	0.10	1.5	[140]
Al_{13}-$(heidi)_6^{3+}$ polycation	type 1/2/3	2.4/6.0/5.2	0/0.38/0.83	12/12.5/25	[141]
$NaAlCO_3(OH)_2$ (dawsonite)		6.70	0.45	10	[142]
$Ca_6Al_2S_3H_{64}O_{50}$	AlO_6	0.36	0.19	13.1	[26]
$Ca_4Al_2SH_{24}O_{22}$	AlO_6	1.7	qp	11.8	[26]
$Ca_6[Al(OH)_6]_2(SO_4)_3·26H_2O$ (ettringite)	Al(1)	0.391	0.164	13.08	[143]
	Al(2)	0.337	0.174	13.51	[143]
$[Al_8(OH)_{14}(H_2O)_{18}](SO_4)_5·16H_2O$	3 sites	3.2/5.75/3.1	0.8/0.1/0.5	4.8/8.4/11.0	[144]
$Al_2(OH)_2(H_2O)_8(SO_4)_2·2H_2O$	AlO_6	4.6	0.4	3	[3]
$Al_2(OH)_4SO_4·7H_2O$ (aluminite)	AlO_6-1/2	10.1/11.6	0.1/0.15	6.9/6.4	[3]
$KAl_3(SO_4)_2(OH)_6$ (alunite)	Al1	10.40	0.05	4.7	[145]
sample A01 from 6 samples	Al_{I1}/ Al_{I2}	-	-	–3.3/0.1	[145]
$KAl(SO_4)_2·12H_2O$	AlO_6	0.400	0.00	–4.1	[32]
$NH_4Al(SO_4)_2·12H_2O$	AlO_6	0.456	0.00	–0.4	[32]
$Ca_4Al_6O_{12}SO_4$ (ye'elimite)	8 sites	2.5-7.6	0.07-0.76	73.6-76.1	[146]

Host compounds

Ca_2SiO_4 larnite (belite)	Al_{IV}	7.1	0.33	96.1	[147]
	Al_{VI}	4.5	0.4	10.1	[147]
	AlO_4	5.8	0.54	94	[148]
MgO periclase	AlO_6	<0.45	-	15.8	[148]

Table 8.2. [23]Na, quadrupole coupling constant $C_\mathrm{Q} = e^2qQ/h$, the asymmetry parameter η, and the isotropic value of the chemical shift δ (referred to 1.0 M NaCl [2]) for the [23]Na NMR of powder inorganic compounds at ambient temperature. An asterisk denotes values of the chemical shift, which were originally referenced to solid NaCl. They are here transformed by the equation δ(referenced to 1M NaCl) = δ(referenced to solid NaCl) + 7.2 ppm. A specification after the reference is a hint to a special selection of data from the source. The acronym "qp" appears in the column for η, if the column C_Q contains the quadrupolar product parameter $P_\mathrm{Q} = C_\mathrm{Q}\sqrt{1+\frac{\eta^2}{3}}$ instead of C_Q.

Compound	site	C_Q/ MHz	η	δ /ppm	Refs.
Silicates without Al					
Na_2SiO_3		1.5	0.7	21.6	[149]
		1.4	0.7	22.1	[150]
		1.46	0.71	22.65*	[151]
$Na_2SiO_3·9H_2O$		1.110	0.63	3.7	[152]
$Na_2SiO_2(OH)_2·8H_2O$		1.14	0.56	3.53*	[151]
$Na_2SiO_2(OH)_2·4H_2O$	Na 1/2	1.80/2.83	0.75/0.17	9.00*/9.50*	[151]
α-$Na_2Si_2O_5$		1.820	1	17.1	[149]
		1.79	1.0	16.9	[153]
		1.82	1	17.1	[154] 132.3 MHz
$Na_2Si_2O_5$, SKS-5, layered, hydrated, site 2		1.6	0.8	0.8	[155]
	site 3/4	0.5/1.2	qp/0.2	–1.0/–0.7	[155]
$Na_2Si_2O_5$, SKS-6, layered, hydrated, site 5/6		1.7/1.6	0.5/0.8	–1.1/0.8	[155]
	site 7/8	1.2/0.6	0.2/ qp	–1.0/–1.0	[155]
δ-$Na_2Si_2O_5$	Na_b 5 c	2.4	1	10	[149]
	site B	2.4	1.0	8.4	[156]
	(2)	2.4	1	9.1	[154] 132.3 MHz
	Na_c 6 c	1.1	0.3	15.9	[149]
	site A	1.1	0.3	15.4	[156]
	(1)	1.16	0.25	16.1	[154] 132.3 MHz
β-$Na_2Si_2O_5$	Na(1)	2.29	0.85	15.6	[153]
	(2)	2.5	0	18.7	[154] 132.3 MHz
	Na(2)	2.20	0.55	9.4	[153]
	(1)	2.22	0.55	9.4	[154] 132.3 MHz
$Na_2O·4SiO_2·5H_2O$ (makatite)	site 1/2/3	1.3/1.5/1.4	0.6/0.4/0.6	0/1/8	[157]
$Na_2O·8SiO_2·9H_2O$ (octosilicate)		0.48	-	–0.7	[157]
$Na_2O·8SiO_2·xH_2O$ (octosilicate dried)		2.4	0.7	–6	[157]
$NaSi_2O_5·3H_2O$ (kanemite)	site 1/2/3	1.7/2.0/0.6	0.7/0.7/-	0/2/–1	[157]
$Na_2Si_{14}O_{29}·11H_2O$ (magadiite)		1.3	0.6	0	[157]
$Na_2Si_{22}O_{41}(OH)_8·6H_2O$ (kenyaite)		0.60	-	–0.5	[157]
$Na_8Si_{12}O_{28}·4H_2O$ (Mu-11)	(A)/ (B)	2.7/2.9	0.4/0.7	1/0.7	[158]
$Na_2BaSi_2O_6$	Na 1/Na 2	2.10/2.96	0.75/0.1	25.0/5.4	[153]
$Na_2H_2SiO_4·8H_2O$		1.11	0.72	3.8*	[159]
$Na_2H_2SiO_4·4H_2O$	(1)/(2)	1.80/2.83	0.75/0.17	9.0*/9.5*	[159]
$10Na_2O$ $10CaO$ $21B_2O_3$ $8Al_2O_3$ $51SiO_2$ (glass)		2.8	0.7	–7.9	[160]
$43.1Na_2O$ $56.9SiO_2$ (glass)		3.0	-	7.5	[161]
Soda-lime silicate glass		1.9	-	4.7	[162]
$Na_4Ti_2Si_8O_{22}·5H_2O$ (penkvilksite)		3.30	0.45	4.3	[163]
Na_3F $SnSi_3O_9$ (stannosilicate)	(A)/ (B)	3.0/3.7	0.55/0.68	12.5/9	[164]

Aluminosilicates / Zeolites / Sodalites

Na-A (dehydrated) near to 6- rings		5.8	0	-	[165]
near to	4, 8-rings	3.2	0.9	-	[165]
Na-LSX (93.2 Na/u.c.)	SI	1.2	0.1	0	[166]
(dehydrated)	SI’	5.9	0.1	–6	[166]
	SII	5.1	0.2	–12	[166]
	SIII’(1,2)	2.2	0.5	–13	[166]
	SIII’(3)	2.0	0.8	–1	[166]
Na-LSX (dehydrated)	SI	1.1	0.5	5.2*	[167]
	SI’	5.8	0.0	–12.8*	[167]
	SII	5.0	0.0	–8.8*	[167]
	SIII’(1,2)	2.2	0.7	–10.8*	[167]
	SIII’(3)	1.2	0.9	–22.8*	[167]
39Li86NaLSX (dehyd.)	SI	1.1	0.5	5.2*	[167]
	SI’	5.4	0.0	–11.8*	[167]
	SII	4.8	0.1	–8.8*	[167]
	SIII’	0	-	–21.8*	[167]
84Li16NaX (dehydr.)	SIII’	0	-	–22.8*	[167]
Na-X (83.5 Na/u.c.)	SI	1.2	0.1	–1	[166]
(dehydrated)	SI’	5.9	0.1	–10	[166]
	SII	4.8	0.2	–16	[166]
	SIII’(1,2)	2.6	0. 5	–17	[166]
	SIII’(3)	2.0	0.8	–11	[166]
Na-X (Si/Al=1.23) MAS/DOR	SI	0/-	0/-	1.2/-*	[168]
(dehydrated)	SI’(1)	5.2/5.0	0/0	–11.8/–12.8*	[168]
	SI’(2)	-/3.6	-/0	-/–20.8*	[168]
	SII	4.6/4.5	0/0.1	–7.8/–10.8*	[168]
	SIII’(1,2)	2.6/3.0	0.7/0.5	–5.8/–3.8*	[168]
	SIII’(3)	1.6/1.9	0.9/0.9	–21.8/–23.8*	[168]
Zeolite Na-X (Si/Al=1.24)	SI	1.4	0	–2.7	[169]
(dehydrated)	SI’	5.4	0	–20	[169]
	SII	4.9	0	–10	[169]
	SIII’(1,2)	3.0	0.5	–11	[169]
	SIII’(3)	2.1	0.9	–21	[169]
Na-Y (Si/Al=2.5) (dehydrated)	SI	0	0	–4.8*	[168]
Na-Y (Si/Al=2.6) (dehydrated)	SI	1.2	qp	–5	[170]
	SI	1.2	0	–1.5	[169]
	SI’	4.8	0	–12	[169]
	SII	3.9	0	–8	[169]
Na-Y (Si/Al=2.7) (dehydrated)	SI	1.2	$0.5_{assumed}$	–3.3*	[171]
	SI’	2.6	$0.5_{assumed}$	–5.4*	[171]
	SII	3.8	$0.5_{assumed}$	–13.0*	[171]
Na-Y (Si/Al=8.6) (dehydrated)	two SI sites	1.1/1.2	$0.5_{assumed}$	–1.2/–6.1*	[171]
	in sodalite c.	1.6	$0.5_{assumed}$	–18.1*	[171]
	SII	3.5	$0.5_{assumed}$	–11.7*	[171]
Na-Y (Si/Al=2.56) (dehydrated)	SI	0.4	qp	–6	[172]
	SI'/SII'	2.3	qp	–12	[172]
	SII	4.2	qp	–4	[172]
	SIII	4.7	qp	5	[172]
Na-Y (Si/Al=2.6) (dehydrated)	SI	1.2	0.1	–3	[166]
	SI’	4.8	0.2	5	[166]
	SII	3.9	0.2	–7	[166]

HNa-Y (21.3 Na/u.c.) (dehyd.)	SI	1.2	0.1	–3	[166]
	SI’	4.9	0.2	5	[166]
	SII	3.8	0.2	–7	[166]
HNa-Y (13.3 Na/u.c.) (dehydr.)	SI	1.2	0.1	–3	[166]
	SI’	4.9	0.3	5	[166]
	SII	3.8	0.2	–7	[166]
HNa-Y (2.7 Na/u.c.) (dehydr.)	SI	1.2	0.1	–3	[166]
	SI’	4.8	0	3.2*	[168]
	SII	3.9	0	–4.8*	[168]
$Ca_{19}Na_{16}$-Y (Si/Al=2.56) (dehy.)	SI	0.4	qp	–2	[172]
	SI’/SII’	2.3	qp	–4	[172]
	SII	4.6	qp	–3	[172]
	SIII	5.0	qp	3	[172]
75Na25K CHA (dehydr.)	SIIa	5.7	qp	–8.1*	[173]
	SIII'a	4.1	qp	–17.5*	[173]
	SIII’b	1.7	qp	–2.8 to –15.6*	[173]
31Li47Na22K CHA (dehy.)	SI	1.2	qp	6.2*	[173]
	SIIa	4.9	qp	–6.8*	[173]
	SIIb	5.3	qp	–4.8*	[173]
	SIII'a	4.1	qp	–17.8*	[173]
	SIII’b	2.0	qp	–3.8 to –13.1*	[173]
64Li13Na23K CHA (dehy.)	SIII'a	4.4	qp	–15.8*	[173]
Na-EMT (Si/Al=3.7) (dehydr.)	SI	1.0	qp	–6.5	[170]
Na-MOR (Si/Al=7.1) (dehydr.)	12-ring	2.0	qp	–14	[170]
	sidepockets	3.1	qp	–24	[170]
Na-ZSM-5 (Si/Al=18) (dehydr.)	10-ring	2.0	qp	–18	[170]
SSZ-13 zeolite (Si/Al=21)	SIIa0/SIIa1	3.1/3.9	0.6/0.2	–11.2/–7.4	[174]
	SIII’a1/SIII’b	2.7/1.8	1/0.6	–20.4/–10.0	[174]
$Na_2Al_2Si_3O_{10}\cdot 2H_2O$ (natrolite)		1.82	0.6	8.18	[175]
$NaAlSi_3O_8$ (albite)		2.69	0.25	–7.1	[176]
$NaAlSi_2O_6$		3.3	0.25	11.0	[153]
Na,K $AlSi_3O_8$ (feldspar)	8 samples	2.136-1.160	0.6-0.7	–20.1-–24.7	[67]
$Na_8Al_2Be_2Si_8O_{24}Cl_2$ (tugtupide)		1.41	0.44	7.7	[64]
$Na(Na_2)Mg_5Si_8O_{22}(OH)_2OH$	M(4)	3.9	0.49	9.3	[69]
(HSMC)	channel (A)	2.9	0.26	5.5	[69]
$Na_{8.0}[AlSiO_4]_6Cl_{1.8}\cdot 0.4\ H_2O$ (NaCl-sodalite)		0.20-0.45	qp	–8.8	[72]
$Na_{7.7}[AlSiO_4]_6Br_{1.8}\cdot 0.4\ H_2O$ (NaBr-sodalite)		0.72	0.12	–9.9	[72]
$Na_{7.8}[AlSiO_4]_6I_{1.7}\cdot 0.4\ H_2O$ (NaI-sodalite)		1.73	0.06	–20.6	[72]
$Na_8Cl_2[Al_6Si_6O_{12}]$ (NaCl-sodalite)		≈0	$0.67_{assumed}$	6.3	[177]
$Na_8B_2[Al_6Si_6O_{12}]$ (NaB-sodalite)		1	$0.67_{assumed}$	8.5	[177]
$Na_8I_2[Al_6Si_6O_{12}]$ (NaI-sodalite)		1.9	$0.67_{assumed}$	9.3	[177]
$Na_8Cl_2[Al_6Si_6O_{24}]$ (NaCl-sodalite)		0.5	qp	6.1	[70]
$Na_8Br_2[Al_6Si_6O_{24}]$ (NaBr-sodalite)		0.7	qp	7.2	[70]
$Na_8I_2[Al_6Si_6O_{24}]$ (NaI-sodalite)		1.8	qp	7.3	[70]
$Na_8[Al_6Si_6O_{24}]\cdot(H_3O_2)_2$ (basic sodalite)		0.8	qp	5	[73]
$Na_8Br_2\ [Al_6Si_6O_{24}]\ \cdot$ (basic sodalite)		0.7	qp	7.5	[73]
$Na_6[Al_6Si_6O_{24}]\cdot(4H_2O)_2$ (hydro sodalite)		1.1	qp	–0.1	[73]
$Na_8Br_2\ [Al_6Si_6O_{24}]$		0.7	qp	7.4	[73]
$Na_6[Al_6Si_6O_{24}]$ (dry sodalite)		5.6	qp	-	[73]
$Na_8Br_2\ [Al_6Si_6O_{24}]$ (dry sodalite)		0.7	qp	7.4	[73]
$Na_6[AlSiO_4]_6$ (anhydrous sodium sodalite)		5.90	0.10	10.2*	[151]
$Na_8[AlSiO_4]_6(OH)_2$ (hydroxosodalite, dehyd.)		2.00	0.10	3.2*	[151]

$Na_8[AlSiO_4]_6(OH)_2·2H_2O$ (hydroxosodalite)		1.55	0.16	–1.2*	[151]
Na-nitride sodalite		1.00	0.18	0.4*	[159]
$Na_8Cl_2(AlSiO_4)_6$ (blue sodalite)		0.081	0.35	95 ?	[71]
$Na_8Si_{12}O_{28}·4H_2O$ (Mu-11)	(A)	2.7	0.4	1	[158]
	(B)	2.9	0.7	0.7	[158]
$Na_6Zn_2[AlSiO_4]_6(SO_4)_2$		1.9	qp	1	[75]
$NaAlSi_2O_6$ (jadeite)		3.30	0.25	11.0	[153]
$(Na_4BH_4)^{3+}$ sodalite	AlSi	8.82	0	–6.61	[178]
	GaSi	6.41	0	–1.31	[178]
	AlGe	6.75	0.22	–1.60	[178]
Al_2O_3-B_2O_3-SiO_2-Na_2O glasses		2.5-3.5	qp	–3-–12	[91]
Soda-lime aluminosilicate glass		1.8	-	–6.9	[162]
$[Na_2O·Li_2O]_{0.46}[0.16Al_2O_3·0.84P_2O_5]_{0.54}$ glass					
	$Al(OP)_6$	2.4-2.6	qp	–10-–11	[179]
	$Al(OP)_5$	3.3-4.0	qp	16-18	[179]
	$Al(OP)_4$	3.4-4.2	qp	46-49	[179]
Nitrogen containing materials					
$NaNO_3$		-	-	–7.3	[180]
		0.337	0.00	–8.0	[32]
$NaNO_2$		1.09	0.11	–0.1	[32]
NaN_3		-	-	–3.5	[180]
		0.297	0.12	–3.8	[32]
Phosphorus containing materials					
$Na_3P_3O_9$	Na 1/Na 2	2.20/1.57	0.70/0.55	–7.60*/1.60*	[151]
$NaPO_3$ glass		2.3	-	–4.2	[114]
60 $NaPO_3$ 40AlF_3 glass		2.2	-	–7.3	[114]
$Na_5P_3O_{10}$ H_2O	1/2	1.74/1.97	0.29/0.85	–0.55/–5.71	[181]
	3/4	2.09/2.40	0.81/0.51	–9.09/2.20	[181]
	5	1.69	0.26	–4.20	[181]
$Na_5P_3O_{10}$	Na 1/ Na 2	4.65/3.06	0.40/0.17		[182]
	Na 3	4.65	0.40		[182]
$Na_2P_2O_7$ H_2O	Na 1/ Na 2	1.37/0.48	0.92/0.99	-	[182]
$Na_4P_2O_7$	Na 1/ Na 2	2.08/2.30	0.26/0.70	5.52/1.96	[183]
	Na 3/ Na 4	2.90/3.22	0.47/0.56	10.41/6.36	[183]
$Na_4P_2O_7$ 10H_2O		-	-	1.5	[180]
$Na_3HP_2O_7$ H_2O	Na 1/ Na 2	2.55/3.60	0.15/0.20	4.0/1.0	[183]
	Na 3	3.1	0.1	6.5	[183]
Na_2HPO_4	Na 1/ Na 2	0.210/0.325	0.18/0.7	–1.4/–2.5	[184]
	Na 3	0.589	0.26	–1.1	[184]
$NaH_2PO_4·2H_2O$		1.19	0.46	2.40*	[151]
$NaH_2PO_4·H_2O$		1.22	0.26	–3.49*	[151]
NaH_2PO_4	Na 1/ Na 2	1.59/2.35	0.46/0.94	-	[182]
$CaNa_4(P_3O_9)_2$	50%/50%	1.405/2.191	0.60/0.69	–3.3/–13.3	[185]
$NaMg(PO_3)_3$	43%/26%	2.67/2.57	0.34/0.47	0.0/–4.3	[186]
	31%	2.72	0.59	–9.8	[186]
$NaZn(PO_3)_3$	41%/28%	2.50/2.66	0.38/0.51	0.0/–4.1	[186]
	31%	2.67	0.59	–9.9	[186]
$NaCa(PO_3)_3$	93%/7%	2.15/0.62	0.88/0.99	3.73/–5.58	[187]
$NaSr(PO_3)_3$		2.38	0.70	2.74	[187]
$NaPO_3$ glass		2.1	qp	–3.4	[188]

$NaPO_3$ glass		2.52	qp	–5.1	[189]
$Na_{0.2}Li_{0.8}PO_3$ glass		2.65	qp	–7.0	[189]
$Na_{0.2}Ag_{0.8}PO_3$ glass		2.41	qp	–5.5	[189]
$Na_{0.22}K_{0.78}PO_3$ glass		2.34	qp	–1.0	[189]
$Na_{0.22}Rb_{0.78}PO_3$ glass		1.93	qp	–0.6	[189]
$Na_{0.19}Cs_{0.81}PO_3$ glass		2.52	qp	–1.7	[189]
$Na_{0.2}Li_{0.8}PO_3$ glass		2.65	qp	–7.0	[189]
$NaPO_3$ –WO_3 glass		2.0	qp	–14.9	[188]
$NaPO_3$– GeO_2 glass		1.8	qp	–4.5	[190]
$(M_2O)_{1/3}[(Ge_2O4)_x(P_2O_5)_{1-x}]_{2/3}$ glass M = Na, K x = 0.0, 0.4, 0.8		1.3/1.7/1.6	qp	–5.7/–8.3/–4.0	[191]
60$NaPO_3$–40MoO_3 glass		2.0	qp	–14.3	[192]
$NaGe_2(PO_4)_3$	site 1/2/3	3.45/3.2/-	0.01/0.02/-	–11.5/–21.7/–37.4	[193]
$Na_{1.4}Al_{0.4}Ti_{1.6}(PO_4)_3$		1.4614	-	–8.3	[194]
$Na_{1.4}Al_{0.4}Zr_{1.6}(PO_4)_3$		1.1200	-	–14.6	[194]
$Ca_{10}K_{0.5}Na_{0.5}(PO_4)_7$		2.4	0.13	–8.8	[195]
$NaSn_2(PO_4)_3$	Na 1/Na 2	2.3/2.5	0/0	-	[196]
$Na_3Fe_3(PO_4)_4$ (layered)	Na 1/Na 2	1.55/1.57	0.03/0.48	277.5/143.0	[197]
$[Na_2O{\cdot}Li_2O]_{0.46}[0.16Al_2O_3{\cdot}0.84P_2O_5]_{0.54}$ glass		1.3	qp	–6	[179]
$Ca_{10}K_{0.5}Na_{0.5}(PO_4)_7$		2.4	0.13	–8.8	[195]
$Ca_{10}Na(PO_4)_7$		2.48	0.2	–5	[198]
$Na_3MnPO_4CO_3$ (sidorenkite)	1/2	1.2/4.4	0.0/0.5	–168/569	[199]
$Na_6[P_2Mo_5O_{23}]$ ·7H_2O	Na(a)/ Na(d)	3.15/2.49	qp/ qp	–1.6/–11.0	[200]
	Na(f)	0.88	qp	–2.1	[200]
HNaPW (hydrated)	1/2	2.0/2.7	1.0/0.0	3/4	[201]
$Na_{15}[(PO_2)_3PNb_9O_{34}]{\cdot}22H_2O$	5 sites	0.63-2.2	0-1	–8.4-3.1	[202]
$Na_5B_2P_3O_{13}$	5 sites	1.54-2.83	0.02-0.85	–7.7-9.2	[203]

Others

Na_4Si_4 (2 at% P-doped)	Na-Si	1.25	1.0	56.7	[204]
	Na-Si	2.31	0.15	49.5	[204]
	Na-P	2.0	0.1	53.3	[204]
Cs_7NaSi_8		5.36	0	72.2	[205]
Rb_7NaSi_8		5.66	0	157.2	[205]
Na_2O		≈0	-	55.1	[206]
Na_2O_2	2 sites	-	-	4.8 and 9.9	[207]
Na_3OCl		11.34	0.0	-	[206]
NaOH	5-coord.	3.59	0.07	21.1	[208]
		3.5	0.00	19.4*	[151]
$NaOH{\cdot}2H_2O$		2.20	0.70	12.2*	[151]
$NaZrO_3$	Na 1/ Na 2	2.52/2.08	0.67/0.05	15.0/27.0	[209]
	Na 3	4.20	0.27	19.5	[209]
$Na_2ZrSi_2O_7$ (parakeldyshite)	Na 1/Na 2	1.5/2.8	1.0/0.85	0.0/2.0	[210]
$Na_2ZrSi_4O_{11}$ (vlasovite)	Na 1/Na 2	1.65/4.70	0.25/0.0	–4.5/–3.0	[210]
$NaZrSi_6O_{15}{\cdot}3H_2O$ (elpidite)	Na 1/Na 2	2.05/2.65	0.50/0.75	–7.0/–1.0	[210]
$Na_4Zr_2Si_3O_{12}$	Na 1/Na 2	2.30/3.10	0.85/0.30	–7.0/9.0	[210]
Na_3GaF_6		1.49	0.4	0.1	[211]
NaF		-	-	7.9	[180]
	octahedr.	≈0	-	7.2	[208]
NaCl		-	-	7.9	[180]
	octahedr.	≈0	-	7.2	[208]
NaBr		-	-	6.0	[180]

	octahedr.	≈0	-	5.1	[208]
NaI				–2.7	[180]
	octahedr.	≈0	-	–3.2	[208]
$NaIO_4$		-	-	–12.5	[180]
Na_2S	tedrahedr.	≈0	-	49.7	[208]
Na_2S	site 1	0	-	49.8	[212]
β-Na_2S_2	site 1/site2	≈0/≈0	-/-	8.5/5.9	[212]
Na_2S_4	site 1/site2	1.03/1.71	0.9/0.7	8.9/3.1	[212]
α-Na_2S_5	site 1/site2	1.87/1.52	0.5/0.3	10.5/0.8	[212]
α-$NaVO_3$	Na 1/ Na 2	1.5/0.765	0.58/0.06	–15.5/–4.8	[213]
β-$NaVO_3$		1.42	0.27	–10.3	[213]
Na_2SO_4		2.60	0.58	–1.3*	[151]
Na_2SO_3	Na 1/ Na 2	1.06/0.33	0.00/0.00	-	[182]
	Na 3	1.14	0.00	-	[182]
$NaAlO_2$		2.15	0.60	26.2*	[151]
$Na[Al(OH)_4]$		3.10	0.00	5.9	[214]
$NaAl_9O_{14}$	1/2	2.15/2.65	0.4/0.2	–15.6/–14.6	[34]
$Na_2Al_2B_2O$	Na 1/Na 2	1.9/0.33	0.1/0	5.5/–7.1	[118]
Na_2B_{29}	50%/50%	2.4/2.2	qp/ qp	10.2/16.9	[215]
$NaBO_2$		1.19	0.24	2.1	[119]
		1.2	0.09	1.8	[216]
$Na_4B_2O_5$	Na 1/Na 2	2.2/3.0	1.0/0.5	19.6/14.4	[216]
$Na_2O{\cdot}4B_2O_3$	Na 1/Na 2	4.1/2.0	0.18/0.35	3.4/ –11.4	[216]
$NaBO_2{\cdot}2H_2O$		1.530	0.80	10.6	[152]
$Na_2B_4O_7$	62%/20%	2.65/1.8	0.91/0.9	–9.9/–12.0	[119]
	18%	1.8	0.1	–4.9	[119]
$Na_2B_4O_7 \cdot 10H_2O$ (borax)	Na 1/Na 2	0.541/0.849	0.499/0.143	-	[217]
$Na_2B_4O_7 \cdot 5H_2O$ (tincalconite)	Na 1/Na 2	0.539/0.785	0.741/0.0	-	[217]
	Na 3	1.299	0.0	-	[217]
$NaCa[B_5O_6(OH)_6]{\cdot}5H_2O$ (ulexite)		0.07	-	7.1	[218]
$H_{15}[Na_4 (V_{12}B_{32}O_{84})]13H_2O$ (polyoxovanadate)	4 sites	0.5-1.8	0.5	–6-15	[219]
$NaSnO_3{\cdot}3H_2O$		1.760	0.00	12.8	[152]
$NaTeO_4{\cdot}2H_2O$		2.240	0.37	12.5	[152]
$Na_2Te_4O_9$	Na 5/Na6	4.4/3.6	0.08/0.12	–3/5	[220]
Na_2TeO_3	Na 1/Na2	1.84/1.36	0.08/0-12	5.8/17.0	[220]
$NaNbO_3$ (polar phase)	Na 1/ Na 2	2.4/1.2	qp/ qp	1.5/–5.1	[221]
$NaNbO_3$ (perovskite)		1.3	0.9	–3.0	[222] MAS
$Li_{0.05}Na_{0.95}NbO_3$	Na 1/ Na 2	1.1/2.3	qp/ qp	–4.6/–0.6	[223]
$NaNbWO_6$	19%/81%	0.4/1.4	0.5/-	–6.5/–18	[224]
$NaTaO_3$ (perovskite)	Na 1/Na 2	2.1/1.0	0.0/0.9	–0.5/–4.5	[222]
Na_2CrO_4	Na 1/Na 2	2.78/0.5	0.57/ qp	–12.8*/–6.7*	[151]
$NaClO_4$		-	-	–20.4	[180]
		0.80	0.35	–18.3*	[151]
$NaClO_4{\cdot}H_2O$	Na 1/Na 2	1.71/1.48	0.20/0.10	–4.5*/–5.2*	[151]
$Na_{1-x}Ge_{3+z}$ ($Na_{0.72}Ge_{3.13}$)	Na6	-	-	20.5	[225]
	Na5(1)/(2)	0.473/0.414	0.25/0.23	4.5/2.4	[225]
$Na_2Ge_2O_5$		2.3	1.0	14.5	[226]
$32Na_2O{\cdot}68GeO_2$ (glass)		3.2	qp	7.9	[226]
$14Na_2O{\cdot}86GeO_2$ (glass)		2.5	qp	–4.1	[227]
Na_2GeO_3		1.3	0.8	22.6	[216]
$Na_4Ge_9O_{20}$		2.7	0.54	–2.1	[216]
$Na_2Ge_4O_9$		2.4	0.7	–6.4	[216]

Na_2MoO_4		2.59	0.00	3.2	[228]
$Na_2MoO_4{\cdot}2H_2O$	Na(1) octah.	0.875	0.23	–1.4	[228]
	Na(2) trig.	2.68	0.08	4.0	[228]
60$NaPO_3$-40MoO_3 (glass)		2.0	qp	–14.3	[192]
Na_3UO_4	site A/B/C	3.4/4.0/2.5	qp	47/18/13	[229]
	site D/E/F	2.6/2.2/2.4	qp	2/–2/–16	[229]
$NaUO_3$		1.7	0.5	–29.2	[230]
Na_4UO_5		3.2	0.2	15.1	[230]
$Na_2U_2O_7$	1/2	1.4/2.0	qp/ qp	–19/–14.1	[230]
Na_2WO_4		2.49	0.00	4.5	[228]
$Na_2WO_4{\cdot}2H_2O$	Na(1) octah.	0.88	0.35	–0.9	[228]
	Na(2) trig.	2.7	0.09	6.3	[228]
Na_2WO_4	(A)	5.2	0.0	–4.0	[231]
	(B)/(C)	small/ small	-	–6/–14	[231]
$[Na_2S]_{2/3}[(B_2S_3)_{1/2}(P_2S_5)_{1/2}]_{1/3}$ (glass)		1.6	qp	3.8	[232]
Na_3AlF_6 (cryolite)	CN 6	0.83	0.62	2.6	[132]
	Na1	0.840	0.6	2	[122]
	CN 8 site 1	1.43	0.27	–8.4	[132]
	Na2	1.430	0.3	–9	[122]
$Na_5Al_3F_{14}$ (chiolite)	Na1/ Na2	1.480/3.180	0.0/0.1	–24/–9	[122]
Na_2MgAlF_7 (weberite)	CN 8 site 1/2	2.48/3.24	0.08/0.26	–28.6/–10.4	[132]
$Na_2Ca_3Al_2F_{14}$		3.360	0	5.2	[133]
α-$NaCaAlF_6$	(i)/ (ii)	2.340/1.360	0.25/0.1	2.0/–1.6	[133]
β-$NaCaAlF_6$		1.200	1	7	[133]
$NaCoO_2$		3.98	0.02	48	[233]
Na_3AlH_6 doped/non-doped site Na1		0.50/0.49	0.6/0.7	23.5/23.3	[46]
Na_3AlH_6 doped/non-doped site Na2		0.93/0.93	0.4/0.4	−8.8/−8.9	[46]
Na_2LiAlH_6		<0.1	-	−17.9	[46]
$NaAlH_4$		0.15	0.2	–9.2	[46]
NaH		<0.1	-	18.2	[46]
$NaHCO_3$				–5.4	[180]
20Na_2CO_3 80γ-Al_2O_3	Na1/Na2/Na3	1.24/2.12/2.45	qp	5.12/0.12/-6,00	[234]
$NaAlCO_3(OH)_2$ (dawsonite)		3.64	0.56	2	[142]
$Na_2C_2O_4$		2.43	0.75	-	[182]
Na_3C_{60}		3.3	0.08	17.2	[235]

Table 8.3. ^{17}O, quadrupole coupling constant $C_Q = e^2qQ/h$, the asymmetry parameter η, and the isotropic value of the chemical shift δ (referred to D_2O [2]) for the ^{17}O NMR of inorganic powder compounds at ambient temperature. For organic compounds, we refer to Wu [236]. Reviews concerning solid-state ^{17}O NMR investigations of inorganic material were presented by Asbrook and Smith [237, 238], Gerothanassis [239], and MacKenzie and Smith [134]. The data in the table, which were published in the years 1989-2000, were compiled by Pingel [240]. sites nb O and br O denote non-bridging and bridging oxygen atoms, respectively. A specification after the reference is a hint to a special selection of data from the reference. The acronym "qp" appears in the column for η, if the column C_Q/ MHz contains the quadrupolar product parameter $P_Q = C_Q\sqrt{1+\frac{\eta^2}{3}}$ instead of C_Q.

Compound	site	C_Q/ MHz	η	δ /ppm	Refs.
Aluminum hydroxides, aluminates					
AlO(OH) (boehmite)	OAl_4	1.20	0.1	70	[241]
	OAl_4	1.15	0.13	70.0	[32]
	Al_2OH	5.0	0.5	40	[241]
$Al(OH)_3$ (bayerite)	Al_2OH	6.0	0.3	40	[241]
α-Al_2O_3 (corundum)	OAl_4	2.17	0.55	75	[241]
	OAl_4	2.13	0.50	72	[12]
	OAl_4	< 2.4	-	66	[242]
γ-Al_2O_3	OAl_4	1.8	qp	73	[241]
	site 1	2.5	-	56.7	[243]
	site 2	0.6	-	68.6	[243]
	site 3	1.1	-	81.0	[243]
	AlO_4	3.5	qp	77.5	[244]
	AlO_5	4.5	qp	37.2	[244]
	AlO_6	4.3	qp	14.0	[244]
BaO/ γ-Al_2O_3	AlO_4	4.5	qp	77.4	[244]
	AlO_5	3.1	qp	34.0	[244]
	AlO_6	4.2	qp	13.7	[244]
η-Al_2O_3	OAl_4	1.6	qp	73	[241]
δ-Al_2O_3	OAl_4	1.6	qp	72	[241]
θ-Al_2O_3	OAl_4	1.2	qp	72	[241]
	OAl_3	4.0	0.6	79	[241]
$Al_{13}O_{40}$ cluster	AlOAl	1.2	0	50	[245]
$NaAlO_2$	AlOAl	1.81	qp	30.9	[246]
$CaAl_2O_4$	nb O	≈1.9	qp	≈141	[246]
	8 br O	1.3-1.9	qp	57.3-86.8	[247]
$CaAl_4O_7$	O1	1.9	0.7	71.6	[247]
	O2 or O3	1.8	0.5	61.5	[247]
	O3 or O2	2.1	0.5	56.8	[247]
	O4	2.5	0.4	40.6	[247]
$LaAlO_3$		1.6 (max.)		170.2	[248]
$Y_3Al_5O_{12}$	OY_2Al_2	1.49	0.99	142	[12]
$Y_4Al_2O_9$	9 sites	1.49	qp	126-372	[12]
$YAlO_3$	$O_{(1)}Y_3Al_2$	1.57	1.00	143	[12]
	$O_{(2)}Y_3Al_2$	1.65	0.35	165	[12]

Silicates without aluminum					
Siliceous zeolite Y, Sil-Y	SiOSi O1	5.1	0.3	42.3	[249]
dehydrated	SiOSi O2	5.39	0.2	37.2	[249]
	SiOSi O3	5.14	0.1	47.3	[249]
	SiOSi O4	5.28	0.2	34.8	[249]
Siliceous ferrierite, Sil-FER	SiOSi 1	5.62	qp	43.1	[250]
dehydrated	SiOSi 2	5.22	qp	41.6	[250]
	SiOSi 3	5.35	qp	40.7	[250]
	SiOSi 4	5.29	qp	39.6	[250]
	SiOSi 5	5.38	qp	39.0	[250]
	SiOSi 6	5.27	qp	37.0	[250]
	SiOSi 7	5.32	qp	37.0	[250]
	SiOSi 8	5.46	qp	35.9	[250]
	SiOSi 9	5.64	qp	34.8	[250]
	SiOSi 10	5.57	qp	28.0	[250]
SiO_2 (low cristobalite)	SiOSi	5.3	0.0	44	[251] MAS
SiO_2 (α-cristobalite)	SiOSi	5.3	0.125	36.7	[252]
		5.35	0.21	37.5	[253]
SiO_2 (α-quartz)	SiOSi	5.21	0.19	43	[253]
SiO_2 (amorphous)	SiOSi	5.8	0.0	50	[254]
	SiOH	4.0	0.3	20	[254]
	SiOH	4.4	0.0	37	[255]
SiO_2 (stishovite)	OSi_3	6.5	0.125	109	[256]
SiO_2 (coesite)	SiOSi O5	5.16	0.292	58	[257]
	SiOSi O2	5.43	0.166	41	[257]
	SiOSi O3	5.45	0.168	57	[257]
	SiOSi O4	5.52	0.169	53	[257]
	SiOSi O1	6.05	0.000	29	[257]
SiO_2 (glass)	SiOSi	5.08	0.150	37.58	[258]
$2Mg_2SiO_4{\cdot}Mg(OH)_2$ (hydr.-chondrodite)	OH	6.6	0.1	25	[259]
$4Mg_2SiO_4{\cdot}Mg(OH)_2$ (hydr.-clinohumite)	OH	7.0	0.2	25	[259]
β-Mg_2SiO_4 (hydr. wadsleyite)	O2	4.9	0.9	76	[260]
		5.0	0.9	78	[261]
	O3	4.4	0.2	66	[260]
	O4	3.8	0.3	65	[260]
	O1	1.3	qp	38	[260]
Mg_2SiO_4 (forsterite)	SiOMg-I	2.35	0.2	61	[262]
		2.8	qp	64	[263]
	O3	2.5	0.2	61	[264] 3QMAS
	SiOMg-II	2.35	1.0	62	[262]
		3.3	qp	72	[263]
	O2	2.5	0.4	64	[264] 3QMAS
	SiOMg-III	2.70	0.3	47	[262]
		3.0	qp	49	[263]
	O1	2.9	0.3	48	[264] 3QMAS
$Mg_3Si_4O_{10}(OH)_2$ (talc)	SiOMg	3.2	0.0	40	[254]
	SiOSi	5.8	0.0	50	[254]
	MgOH	7.3	0.0	0	[254]
$2Mg_2SiO_4{\cdot}Mg(OH)_2$ (chondrodite)	O1/O2	2.5/2.3	0.3/0.2	63/60	[259] 3QMAS
	O3/ O4	2.3/2.7	0.3/0.2	59/52	[259] 3QMAS
$4Mg_2SiO_4{\cdot}Mg(OH)_2$ (clinohumite)	O2/ O6	2.5/2.4	0.3/0.2	65/64	[259] 3QMAS
	O3+O4	2.3	0.1	61	[259] 3QMAS
	O7/ O8	2.4/2.4	0.2/0.2	60/59	[259] 3QMAS

	O5/O1	2.7/2.7	0.2/0.2	52/49	[259] 3QMAS
$MgSiO_3$ (ortoenstatite)	O21/ O22	2.8/2.9	qp/ qp	42/46	[265]
	O11/O12	3.0/3.0	qp/ qp	52/54	[265]
	O31/ O32	4.3/4.9	qp/ qp	64/73	[265]
$MgSiO_3$ (protoenstatite)	O1+impurity	2.8	qp	52	[265]
	O2/ O3	2.7/4.3	qp/ qp	39/66	[265]
$MgSiO_3$ (clinoenstatite)	O21/ O22	2.8/2.8	qp/ qp	45/41	[265]
	O11/ O12	3.0/3.0	qp/ qp	51/54	[265]
	O31/ O32	4.3/4.8	qp/ qp	64/75	[265]
	6 sites	2.9–5.2	qp	57-70	[263]
	SiOMg-I	3.2	0.0	60	[266]
	SiOMg-II	3.2	0.0	42	[266]
	SiOSi	5.1	0.3	62	[266]
$Mg_3Si_4O_{10}(OH)_2$ (talc)	SiOMg	3.2	0.0	40	[254]
	SiOSi	5.8	0.0	50	[254]
	MgOH	7.3	0.0	0	[254]
$CaMgSi_2O_6$ (diopside)	SiOCa	2.7	0.0	84	[266]
	SiOCa	2.83	0.13	86	[263]
	O1	2.7	qp	85	[265] 81.4 MHz
	SiOMg	2.7	0.1	63	[266]
	SiOMg	2.74	0.00	64	[263]
	O2	2.9	qp	63	[265] 81.4 MHz
	SiOSi	4.4	0.3	69	[266]
	SiOSi	4.39	0.36	69	[263]
	O3	4.3	qp	70	[265] 81.4 MHz
α-$CaSiO_3$ (pseudowollastonite)	br O	3.8	0.2	75	[266]
	2 nb O	2.3/2.1	0.1/0.1	91/94	[266]
$CaSiO_3$ (wollastonite)	9 sites	2.0-4.8	qp	67-115	[263]
Ca_2SiO_4 (larnite)	4 sites	2.5-2.9	qp	122-134	[263]
$38.5CaO\cdot61.5SiO_2$ (glass CS46)	nb O	2.1	qp	104.7	[267]
	SiOSi	4.3	qp	62.7	[267]
$Li_2Si_2O_5$	br O1	5.6	0.55	108	[268]
	br O2	4.05	0.05	35	[268]
	nb O3	2.45	0.1	38	[268]
$Li_2Si_2O_5$ (glass)	br O	5.0	0.15	68	[268]
	nb O	2.55	0.2	42	[268]
Na_2SiO_3	br O2	4.20	0.58	63	[150]
	nb O1	2.43	0.17	39	[150]
α-$Na_2Si_2O_5$	br O1/ br O2	5.74/4.67	0.2/0.3	52/74	[268]
	br O1/ br O2	5.7/4.7	0.0/0.25	55/55	[256]
	nb O3	2.4	0.2	36	[268]
		2.35	0.1	34	[256]
ϵ-$Na_2Si_2O_5$	nb O	-	-	45	[256]
$Na_2Si_2O_5$ (glass)	br O	4.9	0.1	69	[268]
	nb O	2.35	0.2	37	[268]
$Na_2Si_4O_9$ (glass)	SiOSi	5.2	0.22	51	[269]
	nb O	2.7	0.25	40	[269]
	H_2O	6.0	0.7	20	[269]
$Na_2Si_3O_7$ (glass)	br O/ nb O	5.0/2.3	0/0	60/39	[256]
$24Na_2O\cdot76SiO_2$ (glass)	SiOSi	4.73	0.5	48.3	[270]
	SiONa	2.03	0.6	32.2	[270]
$Na_8Si_{32}O_{64}(OH)\cdot32H_2O$	SiOSi	5.1	0	42.6	[271]
(sodium ilerite, RUB-18)	SiOH	3.1	0	61.2	[271]

$Na_4Zr_2Si_3O_{12}$	SiOZr 1	2.68	0.0	169.5	[210]
	SiOZr 2	2.75	0.1	118.0	[210]
	SiOZr 3	2.80	0.2	126.0	[210]
$ZrSiO_4$	SiOZr	-	-	160	[210]
$K_2Si_2O_5$	br O1	5.1	0.1	114	[268]
	br O2	4.7	0.2	69	[268]
	nb O3	2.1	0.5	72	[268]
$K_2Si_2O_5$ (glass)	br O	4.7	0.25	60	[268]
	nb O	2.5	0.45	84	[268]
$K_2Si_4O_9$ (wadeite)	br O1	4.45	0.35	62.5	[256]
	SiOSi O2	4.90	0.2	97	[256]
$KHSi_2O_5$	br O	4.9	0.1	51	[272]
	nb O	3.5	0.35	60	[272]
$K_2Si_4O_9$ (glass)	br O	4.9	0	52	[256]
	nb O	2.3	0	76	[256]
$Rb_2Si_2O_5$	br O1	4.4	0.1	124	[268]
	br O2	4.7	0.5	59	[268]
	nb O3	1.9	0.5	93	[268]
$Cs_2Si_2O_5$ (glass)	br O	4.55	0.3	68	[268]
	nb O	3.1	0.55	145	[268]
$BaSiO_3$	br O	3.7	0.4	87	[266]
	nb O	1.6	0.1	159	[266]
	nb O	2.1	0.1	169	[266]
$Ba_2TiSi_2O_8$ (fresnoite)	SiOTi	-	-	190 (anisotr.)	[273]
	SiOSi	3		0 (anisotr.)	[273]
$LiTiOSiO_4$	TiOSi	3.05	0.35	157	[274]
	nb apical OTi	$\approx$0	-	741	[274]
α-$SrSiO_3$	br O	4.1	0.4	80	[266]
	nb O	2.2	0.1	105	[266]
	nb O	2.1	0.1	108	[266]
$La_{9.33}(SiO_4)_6O_2$ (apatite-type)	O1 or O2	0.266	0.6	165	[275]
	O2 or O1	0.305	0.6	214	[275]
	O3	0.264	0.6	194	[275]
	O4	-	-	600	[275]
Soda-lime borosilicate glass	SiOSi	4.91	0.34	48.1	[270]
	SiOB	5.24	0.45	61.9	[270]
	BOB	5.07	0.46	84.3	[270]
	SiONa	2.60	1	35.2	[270]
	SiO(Ca, Na)	4.91	0.89	70.5	[270]
Cesium borosilicate glass,	br O slice 1	qp=4.2	0.6	52.9	[276]
CBS-2-1.5	br O slice 2	qp=4.5	0.3	60.1	[276]
	br O slice 3	qp=4.5	0.3	67.8	[276]
	br O slice 4	qp=4.5	0.6	77.5	[276]
	nb O site 2	qp=2.3	-	123.7	[276]
Cesium borosilicate glass,	SiOSi	qp=5.1	0.4	44.7	[276]
CBS-2-1.5	SiOB	qp=5.6	0.8	67.6	[276]
	BOB	qp=5.4	0.7	98.5	[276]
Sodium borosilicate glass,					
NBS-K0.5R0.25	SiOSi	5.13	qp	42.3	[277]
NBS-K2R0.5	SiOSi	5.08	qp	43.9	[277]
NBS-K4.5R0.75	SiOSi	5.08	qp	44.2	[277]
Barium borosilicate glass	nb BaOSi	2.3	qp	158	[278]
40BaO $30B_2O_3$ $30SiO_2$	nb BaOB	3.6	qp	197	[278]

Ba Si glass	br O	4.0	0.3	78	[279]
Ba Ca Si glass	br O	4.1	0.3	68	[279]
Ca Si glass	br O	4.7	0.3	59	[279]
	br O	4.6	0.0	66	[255]
	nb O	2.1	0.2	110	[255]
$CaTiSiO_5$ (crystalline titanite)	Ti-O-Ti	0.2	≈1	632	[280]
	Si-O-Ti	2.7−3.2	0.1−0.2	166−189	[280]
PbO-SiO_2 glasses	Si-O-Si	4.4-4.1	0.5_{assumed}	74.6-80.2	[281]
$0.60 \leq X_{PbO} \leq 0.71$	Pb-O-Si	2.9	0.5_{assumed}	150.7-151.7	[281]
	Pb-O-Pb	3.1-3.0	0.5_{assumed}	287.5-282.6	[281]
Aluminosilicates and sodalites					
Na-A, dehydrated	SiOAl	3.2	0.2	32	[251] MAS
	SiOAl O1	3.5	qp	43.6	[282] 5QMAS
	SiOAl O2	3.6	qp	31.2	[282] 5QMAS
	SiOAl O3	3.4	qp	40.8	[282] 5QMAS
Na-A, hydrated	SiOAl O1	3.4	0	43.6	[283]
	SiOAl O2	3.4	0	31.0	[283]
	SiOAl O3	3.4	0.25	40.5	[283]
	SiOAl O1	3.4	qp	40.9	[284]
	SiOAl O2	3.6	qp	31.7	[284]
	SiOAl O3	3.4	qp	42.4	[284]
	SiOAl O1	3.5	qp	44	[285] 5QMAS
	SiOAl O2	3.6	qp	31	[285] 5QMAS
	SiOAl O3	3.4	qp	41	[285] 5QMAS
	SiOAl O1	3.5	qp	43.8	[282] 5QMAS
	SiOAl O2	3.6	qp	31.0	[282] 5QMAS
	SiOAl O3	3.4	qp	41.4	[282] 5QMAS
K-A, dehydrated	SiOAl O1	3.7	qp	31.6	[282] 5QMAS
	SiOAl O2	3.7	qp	36.3	[282] 5QMAS
	SiOAl O3	3.5	qp	47.2	[282] 5QMAS
K-A, hydrated	SiOAl O1	3.5	qp	50.9	[282] 5QMAS
	SiOAl O2	3.9	qp	33.9	[282] 5QMAS
	SiOAl O3	3.7	qp	54.8	[282] 5QMAS
Sr-A, hydrated	SiOAl O1	3.7	qp	60.2	[282] 5QMAS
	SiOAl O2	3.9	qp	38.0	[282] 5QMAS
	SiOAl O3	3.6	qp	48.7	[282] 5QMAS
Tl-A, hydrated	SiOAl O1	3.3	qp	60.7	[284]
	SiOAl O2	3.6	qp	53.4	[284]
	SiOAl O3	3.2	qp	75.5	[284]
Na,K-LSX, hydrated	SiOAl O1	3.3	qp	50.6	[284]
	SiOAl O2	3.3	qp	42.1	[284]
	SiOAl O3	3.4	qp	45.2	[284]
	SiOAl O4	3.6	qp	36.8	[284]
Na-LSX, hydrated	SiOSi	5.0	qp	53	[285] 3QMAS
	SiOAl O1	3.2	0.4	50.3	[283]
	SiOAl O1	3.5	qp	49	[285] 5QMAS
	SiOAl O2	3.3	0.3	41.7	[283]
	SiOAl O2	3.3	qp	37	[285] 5QMAS
	SiOAl O3	3.4	0.3	45.0	[283]
	SiOAl O3	3.4	qp	42	[285] 5QMAS
	SiOAl O4	3.6	0.15	36.9	[283]

Na,K-LSX, dehydrated	SiOAl O1	3.2	qp	42.5	[286]
	SiOAl O2	3.3	qp	37.9	[286]
	SiOAl O3	3.3	qp	38.7	[286]
	SiOAl O4	3.3	qp	33.1	[286]
	SiOAl O1	-	-	43.3	[287]
	SiOAl O2	-	-	36.1	[287]
	SiOAl O3	-	-	33.3	[287]
	SiOAl O4	-	-	25.4	[287]
Rb,K-LSX, dehydrated	SiOAl O1	-	-	56.4	[287]
	SiOAl O2	-	-	47.8	[287]
	SiOAl O3	-	-	44.7	[287]
	SiOAl O4	-	-	35.8	[287]
Ga-X	SiOGa	4.0	0.3	28	[288]
	SiOSi	5.0	0.0	50	[288]
	SiOSi	4.6	0.1	44	[251] MAS
Ba, Na-Y, Si/A=2.74, dehydr.	SiOAl	3.4	0.4	40	[251] MAS
	SiOSi	5.1	0.15	52	[251] MAS
Na-Y, dealuminated, dehydr.	SiOSi	5.2	0.2	45	[251] MAS
Na-Y, Si/A=2.74, dehydrated	SiOAl	3.1	0.2	31	[251] MAS
NH_4-Y, Si/A=2.92, dehydr.	SiOAl	3.2	0.2	31	[251] MAS
	SiOSi	5.0	0.1	48	[251] MAS
H-Y, dehydrated	OH δ_{1H}=3.7 ppm	6.0	1.0	21	[289]
	OH δ_{1H}=4.4 ppm	6.2	0.9	24	[289]
	SiO2,3,4-Al	3.7	0.2	27.5	[290]
	SiO1Al	3.5	0.3	33.3	[290]
	SiO2,3,4Si	5.3	0.1	44.0	[290]
	SiO1Si	5.1	0.3	50.0	[290]
Na-ZSM-5, hydrated	SiOSi	5.3	0.12	40.0	[291]
	SiOAl	3.5	0.29	30.0	[291]
H-ZSM-5, dehydrated	OH δ_{1H}=4.2 ppm	7.0	0.75	31	[289]
	OH δ_{1H}=4.2 ppm	6.8	0.5	35	[289]
	OH δ_{1H}=4.2 ppm	5.8	0.6	37	[289]
$Na_6[AlSiO_4]_6\cdot 8H_2O$ (hydrosodalite)	SiOAl	3.4	qp	39.1	[286]
$Na_6[AlSiO_4]_6$ (dehydr. hydrosodalite)	SiOAl	4.3	qp	36.3	[286]
$Na_8[AlSiO_4]_6(OH)_2\cdot 2H_2O$ (hydroxosodalite)		3.4	qp	36.0	[286]
$Na_8[AlSiO_4]_6(OH)_2$ (dehydr. hydroxosodalite)		3.5	qp	39.2	[286]
Ga-sodalite	SiOGa	4.0	0.3	29	[288]
	SiOSi	5.1	0.0	52	[288]
Na-Ba-Ga-sodalite	SiOGa	4.0	0.3	29	[288]
	SiOSi	5.1	0.0	52	[288]
$Na_{0.46}Ca_{2.0}Al_{4.5}Si_{13.5}O_{36}\cdot 10.8H_2O$	SiOSi	5.1	0.18	43	[292]
(stilbite)	SiOAl	3.5	0.28	33	[292]
$NaAlSi_2O_6\cdot H_2O$ (analcime)	SiOSi	5.0	qp	51	[293]
	SiOSi	4.7	qp	51	[285] 5QMAS
	SiOAl	3.1	qp	35	[293]
	SiOAl	3.2	qp	35	[285] 5QMAS
	AlOAl	1.7	qp	26	[293]
	H_2O	6.87	0.67	−15.5	[294]
	H_2O	7.6	0	(−?)18	[295]
$Al_2Si_2O_5(OH)_4$ (kaolinite)	SiOSi O3/O4	4.45/4.75	0.43/0.28	54.3/46.5	[296]
	SiOSi O5	4.65	0.38	51.3	[296]
	OH	6.9	0.55	41.5	[296]
	SiO2Al	3.4	0.8	6	[296]

$KAl_2[(OH,F)_2/AlSi_3O_{10}]$ (muscovite)	SiOSi	4.6	0.5	53.0	[296]
	SiOSi	4.5	qp	53.2	[297]
	SiO2Al	3.5	0.8	66.5	[296]
	SiO2Al	3.5	qp	66.2	[297]
	SiOAl	3.1	0.5	46.2	[296]
	SiOAl	2.89	qp	45.22	[297]
	OH	6.75	0.5	44.5	[296]
	2AlOH	7.4	qp	34	[297]
$NaAlSi_2O_6$ (jadeite)	O1	3.3	0.9	64	[57]
	O2	4.1	0.15	59	[57]
	O3	5.0	0.5	69	[57]
$Mg_3Al_2Si_3O_{12}$ (pyrope)		3.40	0.30	84.0	[57]
$Ca_3Al_2Si_3O_{12}$ (grossular)		4.10	0.40	102.0	[57]
$1.7Al_2O_3{\cdot}SiO_2$ (mullite)	Oc*	2.0	0.4	40.5	[57]
	Oc	3.3	0.1	76	[57]
	Oab and Od	3.3	0.3	58.5	[57]
Yttrium aluminosilicat glass	br O	3.1	-	54	[298]
	nb O			143	[298]
	nb O			210	[298]
Lanthanum aluminosilicat glass	br O	3.1	-	58	[298]
	nb O			178	[298]
$NaAlSi_3O_8$ (glass)	SiOSi	5.1	0.15	49	[299]
	SiOSi	5.2	0.2	40	[269]
	SiOAl	3.2	0.05	33	[299]
	SiOAl	3.8	0.2	25	[269]
Na, $LiAlSiO_4$ (glasses)	SiOSi	≈4.5-5.0	-	≈49-66	[300]
	SiOAl	≈3.0-3.5	-	≈35-42	[300]
	AlOAl	≈1.7-1.9	-	≈18-22	[300]
$14Na_2O{\cdot}4Al_2O_3{\cdot}17B_2O_3{\cdot}65SiO_2$ (glass)	SiOSi	5.1	qp	40	[301]
	SiOB	5.2	qp	57	[301]
	BOB	5.6	qp	62	[301]
	SiOAl	3.6	qp	26	[301]
$CaAl_2Si_2O_8$ (glass)	SiOAl	3.5	-	61	[302]
	nb O	2.9	-	113	[302]
Sodium aluminosilicate glass, NAS, Si/Al=0.7	AlOAl	1.85	qp	19	[246]
Calcium aluminosilicate glass, CAS, Si/Al=0.5	AlOAl	2.4	qp	68	[246]
La, Lu, Sc, Y in aluminosilicate glasses		1.82-3.30	-	140-202	[303]

Phosphorous containing materials

$AlPO_4$-5	AlOP	5.7	0.0	63	[288]
$AlPO_4$-11	AlOP	5.7	0.0	64	[288]
$AlPO_4$-17	AlOP	5.6	0.1	67	[288]
$AlPO_4$-14 as synthesized	AlOP	5.85	0.10	66.8	[304]
	AlOP	5.79	0.13	68.1	[304]
	AlOP	5.82	0.18	75.0	[304]
	AlOP	5.06	0.23	78.8	[304]
	AlOP	4.93	0.41	87.2	[304]
	AlOP	5.27	0.34	97.4	[304]
$AlPO_4$-14 calcined, dehydrated	AlOP	5.86	0.16	59.0	[304]
	AlOP	5.76	0.21	68.8	[304]
SAPO-34	Al-O-Si	3.5/3.6	0.15/0.10	32/36	[305]

	Al-O-P	6.3/6.1	0.45/0.45	67/74	[305]
h-P_2O_5	br POP	7.46	0.60	122	[306]
	nb PO	3.96	0.00	80	[306]
KH_2PO_4		5.2	0.55	92	[307]
$NH_4H_2PO_4$		5.1	0.55	93	[307]
α/β-$Mg_2P_2O_7$	nb O	5.27	0.40	82.9	[308]
$Na_4P_2O_7$	2 nb O	3.90/3.90	0.6/0.6	85.7/81.0	[308]
	br O	3.90	0.55	134.3	[308]
$Ba_2P_2O_7$	nb O	4.19	0.26	141.3	[308]
	2 br O	7.25/6.82	0.15/ qp	142.9/134.9	[308]
Sodium phosphate glass	br POP	7.7	0.35	119.1	[309]
51.7Na_2O 48.3P_2O_5	nb PONa	4.8	0.15	84.1	[309]
NaPON glass	PONa	4.4	0.2	8.0	[310]
	PON-1/2/3/4	4.3-4.4	0.1-0.3	12.2-15.8	[310]
Sodium borophosphate glass	nb NaOP	4.2	qp	83	[311]
	br POP	7.9	qp	120	[311]
	nb NaOB	4.7	qp	61	[311]
	br BOP	7.1	qp	93	[311]
$Ca_5(PO_4)_3(OH)$ (hydroxyapatite)	peak 1/2	4.0/4.1	0.0/0.1	108/115	[307]
$CaHPO_4{\cdot}2H_2O$	peak 1/2	4.2/4.3	0/0	98/96	[307]
$CsH(PO_3H)$	O1/O4	3.8	0.0	155	[312]
	O2/O5	4.4	0.1	129	[312]
	O3/O6	5.9	0.5	100	[312]
Germanium containing materials					
GeO_2 (quartz)	GeO_4	7.3	0.48	70	[313, 314]
	O_{44}	7.05	0.53	49.5	[227]
GeO_2 (rutile)	OGe_3	7.5	0.10	160	[313, 314]
	O_{66}	7.35	0.08	152.2	[227]
GeO_2 (glass)	GeO_4	7.1	0.48	70	[314]
	O_{44}	7.7	qp	42	[227]
$Na_2Ge_2O_5$	nb O	5.95	0.0	38.5	[226]
	O_{44}	6.05	0.6	61	[226]
Na_2GeO_3	GeO_4	5.2	0.5	70	[313]
	O_{44} O1	5.5	0.70	75	[227]
	nb O	2.5	0.5	47	[313]
	nb O1	5.45	0.00	45.5	[227]
$Na_2Ge_4O_9$	O_{44}	5.9	0.54	70.0	[227]
	O_{46} A	5.9	0.48	117.0	[227]
	O_{46} B	5.7	0.48	133.5	[227]
	O_{46} C	6.4	0.65	151.0	[227]
$Na_4Ge_9O_{20}$	O_{44}/ O_{46}	6.4/5.6	0.65/0.88	70.0/117.0	[227]
	O_{666}	3.75	0.05	133.5	[227]
$Na_2O{\cdot}9GeO_2$ (glass)	GeO_4& GeO_6	7.0	0.5	165	[313]
2 9GeO_2 (glass)	GeO_4	6.0	0.5	80	[313]
14$Na_2O{\cdot}$86GeO_2 (glass)	O_{44}	7.0	qp	57	[227]
	O_{45}/O_{46}	7.1	qp	97	[227]
	O_{45}/O_{46}	6.3	qp	144	[227]
27$Na_2O{\cdot}$73GeO_2 (glass)	nb O	5.9	qp	47	[227]
	O_{44}	6.6	qp	64	[227]
	O_{45}/O_{46}	6.8	qp	105	[227]
$LiTiOGeO_4$	TiOGe	4.8	0.22	148	[274]
$HfGeO_4$ (gel)	HfOGe	5.2	0.65	185	[315]

Others

H_2O_2 (solution)		-	-	180	[316]	
(NQR at 1.5 K)		16.31	0.687	-	[317]	
$NaIO_4$		11.19	0.066	250	[318]	19.6 T
KIO_4		10.87	0.032	251	[318]	19.6 T HfO_2 and hafnates
	7 compounds	-	-	237.8-331.9	[315]	
	nb apical OTi	≈0	-	749	[274]	
$KReO_4$ (perrhenate)		1.28	0.25	137	[319]	
NH_4ReO_4 (perrhenate)		1.25	0.16	133	[319]	
TiO_2 (rutile)	TiOTi	1.5	0.87	596.5	[320]	
	TiOTi	< 1.5	-	590	[242]	
(anatase)	TiOTi	< 1.1	-	558	[242]	
Ti2O3 (corundum)	TiOTi	< 2.6	-	503	[242]	
Li_2O_2	LiOLi	18.0	0.00	227	[321]	
Li_2, Ca, Sr, $BaTiO_3$	5 compounds	-	-	372-564	[248]	
Li_2, Na_2, Ca, Sr, $BaZrO_3$	5 compounds	-	-	280-376	[248]	
Li_2, $SrSnO_3$	3 compounds	-	-	85-423	[248]	
$LiNbO_3$		3.4 (maximum)	-	504	[248]	
SiO_2/TiO_2 (gel)	SiOSi	5.1	0.0	42	[322]	
QTiAc: TEOS, $Ti(OPr^i)_4$, AcacH	SiOTi	2.7	0.0	174	[322]	
	SiOTi	3.0	0.0	314	[322]	
	nb OTi_4/ nb OTi_3		-	375/542	[322]	
ZrO_2	tetragonal	< 1.4	-	383	[242]	
	tetragonal	0.26	0.68	384	[323]	
(baddeleyite)	2 monoclinic	< 0.9/< 1.0	-	325/402	[242]	
ZnO (wurtzite)		< 1.4	-	383	[242]	
SnO (litharge)		< 2.3	-	251	[242]	
La_2O_3	hexagonal	< 1.4/2.2	-	469/590	[242]	
HfO_2 (baddeleyite)		< 1.1	-	267/335	[242]	
PbO (litharge)		< 0.9	-	294	[242]	
M_xO_y-PDMS-hybrides	SiOTa	3.0	-	243	[324]	
	nb OTa_2	-	-	440	[324]	
	SiONb	-	-	275	[324]	
	nb ONb_2	-	-	545	[324]	
	SiOTi	3.0	-	332	[324]	
	nb OTi_2	-	-	719	[324]	
	SiOZr	3.4	-	219	[324]	
	nb OZr_3	-	-	402	[324]	
V_2O_5 (crystalline)	O_{1A}	0.9	0.6	1213	[325]	
	O_{1B}	4.0	0.7	400	[325]	
	O_{1C}	3.3	0.6	0	[325]	
$Na_2Al_2B_2O$	O1/ O2	3.7/1.4	0.77/0	65.0/24.5	[118]	
SrB_4O_7	BO	5.50/5.60/5.55	0.25-0.65	79.8/78.2/72.1	[326]	
	Tricluster	6.6	0.2	68.0	[326]	
Sodium aluminoborate glass	AlOAl	1.7	qp	18.6	[327]	
NAB-40-20-40	AlOB	3.7	qp	44.1	[327]	
	AlOB	4.1	qp	62.7	[327]	
	B nb O	4.0	qp	83	[327]	
	BOB	4.8	qp	89	[327]	
	BOB	5.0	qp	95	[327]	
NAB-30-5-65	AlOB	4.3	qp	61.9	[327]	
	B nb O	4.0	qp	83	[327]	
	2 BOB	4.8/5.4	qp/ qp	87.1/96	[327]	

Borate, borosilicate, boroaluminate glasses	SiOSi	5.4 and 4.9	qp	37 and 51	[328]
	BOB	5.5 and 5.1	qp	92 and 82	[328]
	SiOB	5.6	qp	64	[328]
	Si[B]ONa	2.2	qp	35	[328]
	Si[B]OK	2.1	qp	76	[328]
	AlOB	4.1	qp	59	[328]
	Al[B]ONa	1.7	qp	16	[328]
Titania based hybrids	POTi 4	5.2	0.15	152.5	[329]
	POTi 1-2-3	5.3	0.15	215.0	[329]
$Mg(OH)_2$ (brucite)	MgOH	6.8	0	20	[330]
	MgOH	6.8	0.0	25	[259]
$Mg(OH)_2$	MgOH	6.8	0.0	25	[241]
$Ba(ClO_3)_2{\cdot}H_2O$	H_2O	6.8	1.00	22	[307]
$Ba_2In_2O_5$ (brownmillerite)	site A (O1/O3)	5.0	0.2	189	[331]
	site B (O2)	5.8	0.2	146	[331]
$Ba_2In_2O_4(OH)_2$	site A/ site B	4.5/4.1	0.0/0.7	188/173	[332]
	site C/ site D	4.2/4.8	0.5/0.7	152/97	[332]
$LaSiO_2N$ (La-N-wollastonite)	nb OSi	2.4	-	215	[333]
$La_4Si_2O_7N_2$	ionic	≈0	-	575	[333]
	nb OSi	2.4	-	220	[333]
La_4SiAlO_8N	ionic	≈0	-	570	[333]
	nb OAl	1.8	-	311	[333]
	nb OSi	3.1	-	246	[333]
$La_{10}Si_6O_{24}N_2$	ionic	<1	-	596	[333]
$NaNO_2$		11.05	0.58	643	[334]
$Na_2(ONNO_2)$		13.5	0.40	265	[335]
$[HONH_3]Cl$		14.7	0.71	90	[335]
LiOH (NQR)		−7.283	0.07	-	[336]
NaOH (NQR at 77 K))		−7.590	0.07	-	[336]
KOH (NQR at 77 K))		−7.140	0.08	-	[336]
β-$Ba(OH)_2$ (NQR at 77 K))		−7.124	0.07	-	[336]
$Sr(OH)_2$ (NQR at 77 K))		−7.267	0.08	-	[336]
$Ca(OH)_2$		6.5	0.00	62	[307]
CaOH		6.5	0.3	71	[255]
$CaCO_3$		6.97	1	204	[337]
ThO_2		very small		576	[338]
UO_2		very small		717	[338]
NpO_2		very small		475	[338]
PuO_2		very small		54	[338]
AmO_2		very small		−754	[338]
$Y_2Sn_2O_7$	O1	≈0.02	0.14	384.0	[339]
	O2	3.2	0.36	172.5	[339]
$Y_2Ti_2O_7$	O1	≈0.02	0.13	386.1	[339]
	O2	0.7	0.50	454.6	[339]
$La_2Sn_2O_7$	O1	≈0.02	0.20	641.5	[339]
	O2	3.3	0.90	222.0	[339]
α-TeO_2		7.39	0.42	179	[340]
$La_2NiO_{4+\delta}$	8 sites	<4.6/≈4.6	-	532 and 3640-5590	[341]
$Ba(ClO_3)_2{\cdot}H_2O$	H_2O	6.91	0.97	19.7	[342]
$Li_2SO_4{\cdot}H_2O$	H_2O	6.6	0.86	−7.1	[342]
$K_2C_2O_4{\cdot}H_2O$	H_2O	6.62	0.95	1.1	[342]
$NaClO_4{\cdot}H_2O$	H_2O	7.35	0.72	−17	[342]

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