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 (Thomson Reuters). A search in this data base returns for all quadrupolar nuclei the following numbers of publications from 1950 to 2015:

deuterium-2	1435	calcium-43	60	rubidium-85	3	cesium-133	116
lithium-6	256	scandium-45	68	rubidium-87	79	barium-135	2
lithium-7	717	titanium-47/49	34	strontium-87	16	barium-137	9
beryllium-9	26	vanadium-50	0	zirconium-91	24	lanthanum-138	1
boron-10	3	vanadium-51	410	niobium-93	56	lanthanum-139	46
boron-11	247	chromium-53	3	molybdenum-95	54	hafnium-177	0
nitrogen-14	365	manganese-55	25	molybdenum-97	0	hafnium-179	0
oxygen-17	792	cobalt-59	76	technetium-99	16	tantalum-181	2
neon-21	0	nickel-61	2	ruthenium-99	8	rhenium-185/187	8
sodium-23	790	copper-63/65	91	ruthenium-101	0	osmium-189	1
magnesium-25	90	zinc-67	41	palladium-105	0	iridium-191	0
aluminum-27	3584	gallium-69/71	175	indium-113	9	iridium-193	0
sulphur-33	33	germanium-73	17	indium-115	27	gold-197	9
clorine-35/37	102	arsenic-75	21	antimony-121	12	mercury-201	4
potassium-39	54	bromine-79	28	antimony-123	4	bismuth-209	4
potassium-40	0	bromine-81	15	iodine-127	26		
potassium-41	0	krypton-83	2	xenon-131	6		

The search string *PY=1950-2015 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.

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]
	AlO_6-(2)	1.9	0.25	9.1	[5]
γ-$Al(OH)_3$ (gibbsite)	AlO_6-(1)	2.2	qp	11	[6]
	AlO_6-Al(2)	2.2	0.75	10.5	[5]
	AlO_6-(2)	4.5	0.45	12	[6]
	AlO_6-Al(1)	4.7	1.00	17.2	[5]
	AlO_6-I	4.6	0.4	13.6	[7]
	AlO_6-II	2.2	0.7	11.3	[7]
γ-AlO(OH) (boehmite)	AlO_6	-		9 (anisotr.)	[8]
	AlO_6	1.8-2.8	0.5-1.0	12.6	[5]
α-Al_2O_3 (corundum)	AlO_6	2.40	0.01	18.8	[9]
α-Al_2O_3	AlO_6	1.58	qp	10.7	[10]
γ-Al_2O_3 (non-hydrated)	AlO_4	8.5	0.8	68	[11]
	AlO_6	5.5	0.7	13	[11]
γ-Al_2O_3 (rehydrated)	AlO_4	5.1	-	71.5	[12]
	AlO_5	5.1	-	44.0	[12]
	AlO_6	3.55	-	10.0	[12]
κ-Al_2O_3	AlO_4	7.6	0.3	81.5	[13]
	AlO_6-(1)	5.0	-	ca. 13	[13]
	AlO_6-(4)	8.5	-	18	[13]
χ-Al_2O_3 (part. dehydr. gibbsite)	AlO_4	5.0	0.3	71.5	[14]
	AlO_5	2.7	0.3	38.5	[14]
	AlO_6	4.5	0.3	11.5	[14]
θ-Al_2O_3	AlO_4	6.4	0.65	80	[15]
	AlO_6	3.5	0	10.5	[15]
η-, γ-, δ-, θ-Al_2O_3	AlO_4	4.7-5.5	0.4-0.8	74-80	[16]
	AlO_6	3.0-4.0	0.4	11-15	[16]
$CaO{\cdot}6Al_2O_3$	AlO_4	2.0	$0_{assumed}$	65	[17]
	AlO_5	6.7	$0_{assumed}$	27.5	[18]
	AlO_6-(1)	1.5	$0_{assumed}$	9	[17]
	AlO_6-(2)	<1	$0_{assumed}$	16	[17]
$CaO{\cdot}2Al_2O_3$	AlO_4-(1)	6.7	0.8	78	[17]
	AlO_4-(2)	13	0.1	ca. 60	[17]
$CaO{\cdot}Al_2O_3$	AlO_4-(1)	2.7	0.85	80	[17]
	AlO_4-(2)	2.7	0.85	83	[17]
$4CaO{\cdot}3Al_2O_3$	AlO_4	2.4	0.95	80	[17]
$12CaO{\cdot}7Al_2O_3$	AlO_4-(1)	3.7	0.9	79	[17]
	AlO_4-(2)	11	0.2	85	[19]
$3CaO{\cdot}Al_2O_3$	AlO_4	9.7	0.3	85	[19]
	AlO_4-(1)	8.69	0.32	79.5	[20]
	AlO_4-(2)	9.3	0.54	78.25	[20]
$4CaO{\cdot}3Al_2O_3{\cdot}3H_2O$	AlO_4-(1)	1.8	0.5	78	[17]
	AlO_4-(2)	5.4	0.45	79	[17]

$CaAl_4O_7$	AlO_4-(1)	6.25	0.88	75.5	[21]
		6.4	0.90	68.1	[22]
	AlO_4-(2)	9.55	0.82	69.5	[21]
		9.5	0.82	59.1	[22]
$CaAl_{12}O_{19}$	site 1/2	3.2/4.2	0.0/0.0	65.7/20.0	[22]
	site 3/4/5	4.5/-/-	0.9/-/-	18.0/13.6/6.7	[22]
	site 1/2	0.15/21.4	-/0.00	16.25/55.8	[23]
	site 3/4/5	3.1/1.6/4.8	0.00/-/0.7	68.1/9.92/22.3	[23]
$SrAl_{12}O_{19}$	site 1/2	0.25/20.75	-/0.00	16.72/57.8	[23]
	site 3/4/5	3.45/1.35/4.9	0.00/-/0.65	67.5/9.45/22.1	[23]
	AlO_4/ AlO_4-d	3.455/20.71	0.5/0.00	67.90/56.91	[24]
	AlO_5	2.590	qp	19.50	[24]
	AlO_6-1/2	17.50/10.06	qp/qp	17.50/10.06	[24]
	AlO_6-3	4.990	0.65	21.73	[24]
$LaSrAl_3O_7$	site 1	3.0	0.5	75.4	[25]
	site 2	6.8	0.5	83.3	[25]
$LaSrAl_{1.5}Ga_{1.5}O_7$	site 1	4.2	0.5	78.7	[25]
	site 2	7.0	0.5	83.8	[25]
$CaAl_2O_4$	AlO_4-(1-5)	2.4-4.2	0.2-0.95	81.2-86.2	[21]
$Ca_{12}Al_{14}O_{33}$	AlO_4-(1)/(2)	9.7/3.8	0.4/0.7	85.9/80.2	[21]
$Ca_3Al_2O_6$	AlO_4-(1)/(2)	8.69/9.3	0.32/0.54	79.5/78.3	[21]
$CaAl_2H_{20}O_{14}$	AlO_6	2.4	qp	10.2	[21]
$Ca_3Al_2H_{12}O_{12}$	AlO_6	0.705	0.09	12.36	[21]
$Ca_4Al_2H_{26}O_{20}$	AlO_6	1.8	qp	10.2	[21]
$KAlO_2$	AlO_4	1.1	0.7	76	[19]
$KAlO_2{\cdot}0.5H_2O$	AlO_4	5.6	0.0	77	[19]
$KAlO_2{\cdot}H_2O$	AlO_4	6.5	0.6	83	[19]
$KAlO_2{\cdot}1.5H_2O$	AlO_4	5.0	0.25	81	[19]
$5BaO{\cdot}Al_2O_3$	AlO_4	2.3	0.8	80	[19]
$BaO{\cdot}Al_2O_3$	AlO_4	2.4	0.4	78	[19]
α-$BaO{\cdot}Al_2O_3{\cdot}2H_2O$	AlO_4-(1)/(2)	3.4/5.1	0.5/0.9	81/80	[19]
α-$LiAlO_2$	AlO_6	2.8	0.05	16	[26]
β-$LiAlO_2$	AlO_4	1.8	0.55	82	[26]
	AlO_4	1.86	0.56	83.0	[27]
γ-$LiAlO_2$	AlO_4	3.2	0.7	81	[26]
β-$NaAlO_2$	AlO_4	1.4	0.5	80	[19]
$NaAl_9O_{14}$	AlO_4	3.4	qp	55.9	[28]
	AlO_6	2.8	qp	9	[28]
$AlCl_3{\cdot}3Al(OH)_3{\cdot}6H_2O$	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	[29]
$Al_2Ge_2O_7$	AlO_5	8.8	0.4	36	[30]
$AlLaGe_2O_7$	AlO_5	7.2	0.37	36	[30]
$Al_2(MoO_4)_3$	AlO_6-(1)/(2)	1.12/0.88	0.65/0.95	−12.4/−13.4	[31]
	AlO_6-(3)/(4)	1.21/0.78	1.0/0.8	−10.3/−11.1	[31]
$MgAl_2O_4$ (spinel)	AlO_4	3.2	0.50	76.5	[32]
	AlO_6-1	3.73	0.26	14.5	[32]
	AlO_6-2	4.46	0.4	−1.0	[32]
$Cd_8(AlO_2)_{12}S_2$ (sodalite)	AlO_4	2.00	< 0.1	80.4	[33]
$Ca_8(AlO_2)_{12}S_2$ (sodalite)	AlO_4	3.55	< 0.1	79.1	[33]
$Cd_8(AlO_2)_{12}Se_2$ (sodalite)	AlO_4	3.95	< 0.1	78.7	[33]
$Cd_8(AlO_2)_{12}(SO_4)_2$ (sodalite)	AlO_4	3.24	< 0.1	79.1	[33]
$Sr_8(AlO_2)_{12}S_2$ (sodalite)	AlO_4	4.65	< 0.1	76.9	[33]

$Sr_8(AlO_2)_{12}Se_2$ (sodalite)	AlO_4	5.10	< 0.1	76.6	[33]
$Sr_8(AlO_2)_{12}(CrO_4)_2$ (sodalite)	AlO_4	6.75	< 0.1	75.5	[33]
$SrAl_{12}O_{19}$	AlO_4	3.45	0.1	68.0	[34]
	AlO_5	2.1	0.7	18.0	[34]
	AlO_6-(1)	0.6	1	17.1	[34]
	AlO_6-(2)	1.3	1	9.6	[34]
	AlO_6-(3)	4.9	0.63	21.7	[34]
$Sr_4Al_{14}O_{25}$	Al1/Al2/Al3	4.4/5.2/4.2	0.8/0.8/0.2	78/82/77	[35]
	Al4/Al5/Al5	2.4/6.8/9.2	0.1/0.2/0.0	12/12/11	[35]
$YAlO_3$	AlO_6	1.61	qp	10.7	[10]
$Y_4Al_2O_9$	AlO_4-1	10.81	0.48	78.2	[10]
	AlO_4-2	10.36	0.77	76.2	[10]
$Y_3Al_5O_{12}$	AlO_6	1.13	qp	2.1	[10]
	AlO_4	6.21	0.05	77.5	[10]
	AlO_6	1.13	qp	2.1	[10]
$Y_3Al_5O_{12}$ (YAG II 800)	AlO_6/AlO_5	-	-	1.2/23.6	[36]
	AlO_4	6.0	0.08	76.6	[36]
$Y_3Al_5O_{12}$ (YAG)	AlO_6	0.6	-	5.38	[37]
	AlO_4	6.1	-	82	[37]
$AlVO_4$	Al1	1.64	0.30	−8.9	[38]
	Al2	6.73	0.42	27.2	[38]
	Al3	5.88	0.58	−1.1	[38]
ZrO_2-Al_2O_3 (co-hydrolysis,	AlO_4/ AlO_5	10.0/5.0	-	78/37	[39]
annealed at 1000 °C)	AlO_6	7.0	-	16	[39]
MgO-Al_2O_3 (annealed at 600 °C)	AlO_4	10.5	-	82	[39]
	AlO_5	10.0	-	41	[39]
	AlO_6	7.0/2.0	-	17/15	[39]
Na_3AlH_6 doped/non-doped		0.52/0.70	0.5/0.2	−42.7/−42.5	[40]
Na_2LiAlH_6		<0.1	-	−46	[40]
$NaAlH_4$		3.15	0.04	97.5	[40]
ZrNiAl	Al-Ni	3.3	0.42	393	[41]
Aluminosilicates					
$Al_2Si_2O_5(OH)_4$ (kaolinite)	AlO_6	3.6	qp	7	[6]
	AlO_6 (1)/(2)	3.4/3.0	0.8/0.9	7.5/8.0	[42]
Al_2SiO_5 (sillimanite)	AlO_4	6.77	0.53	64.5	[43]
	AlO_4	6.74	0.51	63.9	[44]
	AlO_6	8.93	0.46	4.0	[43]
	AlO_6	8.83	0.49	4.7	[44]
Al_2SiO_5 (andalusite)	AlO_5	5.6	0.76	35.2	[45]
	AlO_6	15.3	0.13	11.9	[45]
Al_2SiO_5 (kyanite)	AlO_6-(1)/(2)	10.1/3.8	0.27/0.85	13.0/4.0	[45]
	AlO_6-(3)/(4)	6.4/9.2	0.70/0.38	5.7/5.9	[45]
$Al_4Si_8O_{20}(OH)_4$ (pyrophillite)	AlO_6			4.3	[46]
dehydroxylate (550 °C)	AlO_5	10.5	0.6	29	[46]
$K_{1.5}Al_4(Si_{6.5}Al_{1.5})O_{20}(OH)_4$ (illite)	AlO_4	2.9	-	72.4	[47]
	AlO_6	3.7	-	6.0	[47]
$3Al_2O_3{\cdot}SiO_2$ (mullite)	AlO_6	7.3	0	6.3	[48]
	AlO_4 (T)/(T')	7.3/6	0/0.5	68/53	[48]
	AlO_4 (T*)	4	0.5	45	[48]
$2Al_2O_3{\cdot}SiO_2$ (2:1 mullite)	AlO_6 site 1	4.5	qp	7.5	[49]
	site 2	3.2	qp	49	[49]
	AlO_4 site 3	4.6	qp	69.4	[49]

$3Al_2O_3{\cdot}2SiO_2$ (mullite precursor	site 1a/1b	4.3/3.4	qp/qp	7/15	[50]
obtained by sol-gel synthesis)	site 2	4.3	qp	37	[50]
	site 3	4.1	qp	71	[50]
$Mg_3Al_2Si_3O_{12}$ (pyrope)		1.0	0.5	2.9	[51]
$Ca_3Al_2Si_3O_{12}$ (grossular)		3.7	0.2	−3.35	[51]
$Ca_2Al_3Si_3O_{12}$-(OH) (zoisite)	AlO_6 1/2	7.9/18.4	0.51/0.16	10.7/8.0	[52]
	AlO_6 1/2	8.0/18.19	0.53/0.13	10.7/7	[53]
$CaAlAlSiO_6$ (clinopyroxene)	AlO_6 a/b/c	5.0/4.6/5.6	0.5/0.7/0.7	2.7/8.6/13.5	[54]
	AlO_4 d/e	5.4/11.8	0.5/0.45	66.5/79.7	[54]
$Sr_3Al_{10}SiO_{20}$	Al(1)	3.73	0	7.2	[55]
	Al(2)	8.13	0.3	12.0	[55]
	T_2(4Al)	2.61	0	82.0	[55]
	T_1+T_2(*n*Al, *m*Si)	6.86	0.3	78.0	[55]
$(Mg,Fe,Al)_6(Si,Al)_4O_{11}(OH)_8$	AlO_4	2.8	-	72	[43]
(pennine, penninite)	AlO_6	1.4	-	10	[43]
$KAlSi_2O_6$ (leucite)	T1/T2/T3	2.07/2.58/2.34	qp	61.0/63.9/69.2	[56]
$CaAl_2Si_2O_8$ (anorthite)	6 sites	2.7−8.2	0.45-0.70	61-66	[56]
$Na_{16}Ca_{16}$ $(AlO_2)_{48}(SiO_2)_{72}$ (mesolite)	Al(1)	3.0	0	64.4	[57]
	Al(2)	1.9	0	62.6	[57]
	Al(3)	2.0	0	65.1	[57]
$KAl_2[(OH,F)_2/AlSi_3O_{10}]$	AlO_4	2.1	-	72	[43]
(muscovite)	AlO_6	2.2	-	5	[43]
$CaAl_2[(OH)_2/Al_2Si_2O_{10}]$	AlO_4	4.2	-	76	[43]
(margarite)	AlO_6	6.3	-	11	[43]
$CaMg_3Al_2Si_2O_{10}(OH)_2$	AlO_4	2.8	-	76	[43]
(xantophyllite)	AlO_6	2.0	-	11	[43]
$Na_8Al_2Be_2Si_8O_{24}Cl_2$ (tugtupite)	AlO_4	1.36	0.08	63.4	[58]
$NaAlSi_3O_8$ (low albite)	AlO_4	3.29	0.62	62.7	[59]
$Na_2Al_2Si_3O_{10}{\cdot}2H_2O$ (natrolite)	AlO_4	1.67	0.50	64	[43]
$Na_2Al_2Si_3O_{10}{\cdot}2H_2O$ (tetranatrolite)	AlO_4 T1/T2	2.2/2.4	qp/qp	63.1/64.2	[60]
$KAlSi_3O_8$ (microcline)	AlO_4	3.22	0.21	58.5	[59]
Na,K $AlSi_3O_8$ (feldspar)	8 samples	3.15-4.0	0.25-0.52	59.2-61.0	[61]
(Mg, Fe)Al_3SiBO_9 (grandidierite)	AlO_5	8.7	0.95	41.0	[62]
	AlO_6-(1)/(2)	3.5/8.6	0.5/0.95	9.0/11.0	[62]
$NaCa_2Mg_4Al(Si_6Al_2)O_{22}(OH)_2$ (pargasite)	AlO_4 (Q^3)	4.0	qp	77	[63]
$NaCa_2Mg_5Al(Si_7Al)O_{22}F_2$	AlO_4 (Q^2)	3.0	qp	76	[63]
(fluor edenite)	AlO_4 (Q^3)	5.9	qp	77	[63]
$Na_8Cl_2[Al_6Si_6O_{24}]$ (NaCl-sodalite)		0.7	qp	64.7	[64]
$Na_8Cl_2[Al_6Si_6O_{24}]$ (blue sodalite)	AlO_4	1.45	0.1	40	[65]
$Na_{8.0}Cl_{1.8}[AlSiO_4]_6$ ·0.4 H_20	AlO_4	0.94	0.32	62.9	[66]
$Na_8Br_2[Al_6Si_6O_{24}]$ (NaBr-sodalite)		0.8	qp	63.2	[64]
$Na_8I_2[Al_6Si_6O_{24}]$ (NaI-sodalite)		0.6	qp	61.2	[64]
$Na_8[Al_6Si_6O_{24}]{\cdot}(H_3O_2)_2$ (basic sodalite)		0.8	qp	64.5	[67]
Na_8Br_2 $[Al_6Si_6O_{24}]$ · (basic sodalite)		0.8	qp	63.4	[67]
$Na_{7.7}Br_{1.8}[AlSiO_4]_6$ ·0.4 H_20	AlO_4	0.81	0.29	61.8	[66]
$Na_6[Al_6Si_6O_{24}]{\cdot}(4H_2O)_2$ (hydro sodalite)		2.2	qp	65.6	[67]
Na_8Br_2 $[Al_6Si_6O_{24}]$ (dry sodalite)		0.8	qp	63.4	[67]
$Li_{7.6}Na_{0.4}Cl_{1.9}[AlSiO_4]_6$ ·0.7 H_20	AlO_4	0.98	0.59	71.9	[66]
$Li_{7.3}Na_{0.3}Br_{1.8}[AlSiO_4]_6$ ·1.1 H_20	AlO_4	0.71	0.61	70.9	[66]
$Na_{7.8}I_{1.7}[AlSiO_4]_6$ ·0.6 H_20	AlO_4	0.57	0.34	60.4	[66]
$Ca_8(OH)_8Al_8Si_4O_{24}$ (sodalite)	AlO_4	5.3	0.24	-	[68]
Na_6 $[AlSiO_4]_6$ (sodalite)		2.7	$0_{assumed}$	54	[69]

$Na_6Zn_2[AlSiO_4]_6(SO_4)_2$ (sodalite)		2.5	$0_{assumed}$	58	[69]
Zeolite Na-A (hydrated)	AlO_4	1.1	0.75	59.2	[43]
Zeolite Na-Y (hydrated)	AlO_4	2.0	0.5	62.8	[43]
Zeolite Na-Y (dehydrated)	AlO_4	5.5	0.3	ca. 60	[70]
Zeolite H-Y (dehydrated)	AlO_3	13.1	0.75	105±20	[70]
	AlO_3	15.3	0.4	60	[71]
Zeolite Al, Na-Y (dehydrated)	AlO_4/Al^{x+}	14.5	0.3	70	[11]
	AlO_4/Na^+	5.5	0.8	60	[11]
	Al^{x+}cat.	6.0	0.7	35	[11]
Zeolite H, Na-Y (hydrated)	AlO_4/H^+	16.0/14.0	0.3	70	[11]
	AlO_4/Na^+	5.5	0.8	60	[11]
Dealumin. H, Na-Y (hydr.)	AlO_4/H^+	15.0	0.3	70	[11]
	AlO_4/Na^+	8.0	0.8	65	[11]
	Al^{x+}cat.	7.5	0.7	35	[11]
	AlO_6 cluster	5.0	0.7	10	[11]
Zeolite USY (hydrated)	AlO_4	2.8	-	60.0	[12]
	AlO_5	4.1	-	34.5	[12]
	AlO_6	2.9	-	4.0	[12]
	AlO_4 (4 sampl.)	1.9-7.5	qp	60.5-69.7	[72]
	AlO_5 (4 sampl.)	3.9-4.6	qp	34.0-39.8	[72]
	AlO_6 (4 sampl.)	1.9-3.2	qp	0.1-7.5	[72]
Zeolite Ti-USY	AlO_4	2.0/1.5	qp/qp	64.4/61.1	[73]
	AlO_5	3.2	qp	33.9	[73]
	AlO_6	2.0/1.6	qp/qp	6.0/0.01	[73]
Zeolite H-MOR (dehydrated)	AlO_3	15.0	0.35	-	[74]
	AlO_4	6.8	0.7	-	[74]
Zeolite NH_3(H)-MOR	$AlO_4(NH_4)/(H)$	1.9/5.6	qp/ qp	45/35	[75]
Zeolite Beta (Si/Al=9-215)	Td1	2.3-2.5	qp	57.5-59.0	[76]
	Td2	1.7-1.9	qp	53.5-54.0	[76]
Zeolite H-Beta (Si/Al=9-215)	Td1	1.0-2.0	qp	58.5-60.0	[76]
	Td2	1.1-1.7	qp	55.0-60.0	[76]
Zeolite BEA (3 samples)	AlO_4 (2b)	2.3-2.4	qp	58.0-58.4	[77]
	AlO_4 (2a)	1.5-1.8	qp	53.9-54.2	[77]
	AlO_6	-	-	∼0	[77]
Zeolite Na-ZSM-5 (dehydrated)	AlO_4	4.7	0.5	ca. 60	[70]
Zeolite H-ZSM-5 (dehydrated)	AlO_3	16.0	0.1	82±20	[70]
	AlO_3	15.5	0.5	-	[74]
	AlO_4	7.3	0.7	-	[74]
Zeolite ZSM-5 Si/Al=14-250, 7 samples					
	AlO_4, Peak I	1.6-1.7	qp	54.4-55.7	[78]
	AlO_4, Peak II	1.5-1.6	qp	52.2-52.3	[78]
Zeolite TPA-ZSM-5	AlO_4 (1)/(2)	1.4/1.8	qp/ qp	52.2/54.9	[79]
Zeolite H-ZSM-5	AlO_4(1)/(2)	1.2/1.6	qp/ qp	55.5/56.5	[79]
Zeolite NH_3(H)-ZSM-5	AlO_4(1)/(2)	1.2/1.6	qp/ qp	53.8/56.4	[79]
H, Al-MCM-41 (as synthesized)	AlO_4	2.3	$0_{assumed}$	52.6	[80]
Al_2O_3-B_2O_3-SiO_2-Na_2O glasses		3.7-4.2	qp	59-63	[81]
$0.5Al_2O_3$–$xSiO_2$ glasses	AlO_4	5.3-6.5	qp	59-68	[82]
with $1 \leq x \leq 6$	AlO_5	4.6-5.3	qp	32-37	[82]
	AlO_6	3.9-4.6	qp	3-6	[82]
Na_2O-CaO-Al_2O_3-SiO_2 glass ANCS	AlO_4	6.8	-	60.5	[83]
	AlO_5	7.4	-	34.7	[83]

Phosphorous containing materials

$AlPO_4$ (quartz)	AlO_4	4.2	0.35	44.8	[84]
$AlPO_4$ (tridimite)	AlO_4	0.75	0.95	39.8	[84]
$AlPO_4$ (cristobalite)	AlO_4	1.2	0.75	42.5	[84]
$Al_2PO_4(OH)_3$ (augelite)	AlO_5	5.5	0.78	30	[85]
	AlO_6	4.7	0.2	−3	[85]
$Al_2PO_4(OH)_3 \cdot H_2O$ (senegalite)	AlO_5	2.87	$0_{assumed}$	30	[85]
	AlO_6	4.09	$0_{assumed}$	1.7	[85]
$KAlP_2O_7$	AlO_6	1.2	0.25	−16	[86]
$Zn_3Al_6(PO_4)_{12}$	site 1	1.6	0.4	49.74	[87]
	site 2	1.233	0.6	47.6	[87]
$AlPO_4$-5 (hydrated)	AlO_4	2.3	0.95	40.4	[84]
$AlPO_4$-8 (dehydrated)	AlO_4-(1)/(2)	3.9/3.6	$0.5_{ass.}$/ $0.5_{ass.}$	40.1/40.6	[88]
	AlO_4-(3)/(4)	3.6/3.0	$0.5_{ass.}$/ $0.5_{ass.}$	47.0/42.9	[88]
	AlO_4-(5)	3.4	$0.5_{assumed}$	42.6	[88]
$AlPO_4$-14 (hydrated)	AlO_5-(Al1[89])	5.66	0.89	27.2	[90]
	AlO_5-(3)(Al1[89])	5.58	0.97	27.1	[91]
	AlO_5-Al1	5.6	1.0	27	[92]
	AlO_4-(Al2 [89])	4.15	0.82	44.0	[90]
	AlO_4-(2)(Al2 [89])	4.08	0.82	43.5	[91]
	AlO_4-Al2	4.1	0.8	44	[92]
	AlO_4-(Al3 [89])	1.75	0.70	43.2	[90]
	AlO_4-(1)(Al3 [89])	1.74	0.63	42.9	[91]
	AlO_4-Al3	1.7	0.6	43	[92]
	AlO_6-(Al4 [89])	2.60	0.68	−0.9	[90]
	AlO_6-(5)(Al4 [89])	2.57	0.7	−1.3	[91]
	AlO_4-Al4	2.6	0.7	−1	[92]
$AlPO_4$-14 (dehydrated)	AlO_4-Al1	4.0	0.8	43	[92]
	AlO_4-Al2	3.4	0.2	43	[92]
	AlO_4-Al3	2.5	0.6	38	[92]
	AlO_4-Al4	4.9	0.3	45	[92]
$AlPO_4$-14A (dehydrated)	AlO_4-Al1	4.5	-	63.4	[93]
	AlO_4-Al2	4.1	-	43.1	[93]
	AlO_4-Al3	4.7	-	45.5	[93]
	AlO_4-Al4	2.6	-	−14.9	[93]
$AlPO_4$-15	Al1	3.1	0.8	2.5	[94]
	Al2	3.1	0.8	−5.0	[94]
$AlPO_4$-21 (hydrated)	AlO_4	8.3	0.15	47.3	[95]
	AlO_5-(1)/(2)	5.9/7.4	0.68/0.52	14.6/15.7	[95]
$AlPO_4$-25 (hydrated)	AlO_4-(1)/(2)	1.9/0.8	$0.67_{ass.}$/$0.67_{ass.}$	40.8/39.5	[95]
$AlPO_4$-25 (dehydrated)	AlO_4-(1)	2.3/1.1	$0.67_{ass.}$/$0.67_{ass.}$	39.2/37.5	[95]
$AlPO_4$-53 (hydr. and dehydr.)	sites Al1-Al6	2.0-9.2	0-0.9	17-45	[96]
$AlPO_4$-ZON	site Al1	3.8	qp	50.6	[97]
	site Al2	3.6	qp	43.0	[97]
	site Al3	4.9	qp	27.2	[97]
	site Al4	6.3	qp	24	[97]
$AlPO_4$-SOD as-synthesized	Al1/2/3	2.3/2.4/2.7	0.79/0.79/0.82	38/41/−8.5	[82]
dehydrated at 200 °C	Al1/2/3	2.6/2.8/2.6	0.99/0.42/0.92	39/37/36	[82]
	Al4/5	2.7/2.4	0.35/0.98	12/−12	[82]
$AlPO_4$-STA-2	Al1/Al2	2.0/3.5	0.7/0.9	36.0/42.0	[98]
	AlO_4 3 sites	2.4/3.6/2.1	qp/qp/qp	39/45/49	[99]
	AlO_5	3.1	qp	17	[99]
Layered aluminophosphates	6 sites	1,3-5.8	0.1-1.0	−17.6-48.1	[100]
$xAl_2O_3 \cdot (30-x)P_2O_5 \cdot 70SiO_2$	AlO_4	4.0-6.3	qp	40.1-61.5	[101]

x=2.5-27.5% (glass)	AlO_5	4.0-6.0	qp	9.4-35.0	[101]
	AlO_6	4.0-5.0	qp	−20.4-5.0	[101]
$AlPW_{12}O_{40}$ dehydrated at 473 K	AlO_6	2.4/6.0	1/0.8	2/4	[102]
	AlO_5	7.0/8.7	0.2/0.2	24/44	[102]
	AlO_4	8.5	0.8	65	[102]
Boron containing materials					
$2SrO{\cdot}Al_2O_3{\cdot}B_2O_3$	AlO_4	4.3	0.65	83.5	[103]
$2CaO{\cdot}Al_2O_3{\cdot}B_2O_3$	AlO_4	6.25	0.45	79.5	[103]
$2Li_2O{\cdot}Al_2O_3{\cdot}B_2O_3$	AlO_4	6.0	0.45	76	[103]
$3Li_2O{\cdot}Al_2O_3{\cdot}2B_2O_3$	AlO_4	6.7	0.83	70	[103]
$9Al_2O_3{\cdot}2B_2O_3$	AlO_4	6.8	0.1	53	[103]
	AlO_5	4.8	0.3	31	[103]
	AlO_6	6.2	0.4	10.5	[103]
$Al_{6-x}B_xO_9$ (mullite structure)	$AlO_{4\ or\ 5}$	3.9-9.0	-	33.0-67.8	[104]
8 samples with $1 \leq x \leq 4$	AlO_6	4.0-10.5	-	5.1-21.9	[104]
$Na_2Al_2B_2O$	AlO_4	1.65	0.05	70.3	[105]
$Li_6Al_2(BO_3)_4$		6.4	0.88	69.3	[106]
Flour containing materials					
AlF_6^{3-} octahedrons, fluoroaluminates		0.065-1.58	0-0.95	−7-1	[107, 108]
AlF_3		0.213	0.0	-	[109]
α-AlF_3	AlF_6	2.8	0	−13.2	[110]
β-AlF_3	AlF_6	3.4	0	−12.5	[110]
β-$AlF_{6-x}(OH)_x$ (82 $m^2\ g^{-1}$)	AlF_6 and $AlF_5(OH)$	0.28	qp	−15.5	[111]
	$AlF_4(OH)_2$	0.61	qp	−11.7	[111]
	$AlF_3(OH)_3$	0.990	qp	−9.5	[111]
HS-AlF_3	site A/B	3.88/8.68	qp/qp	4.8/−7.9	[112]
	site C/D	6.37/5.04	qp/qp	−7.4/−7.7	[112]
$H_3AlF_6{\cdot}6H_2O$	AlF_6	0.3	0.0	−2.8	[113]
$K_2AlF_5{\cdot}H_2O$	AlF_6	12	0.0	0	[113]
$Rb_2AlF_5{\cdot}H_2O$	AlF_6	13	0.0	0	[113]
$CsAlF_5{\cdot}H_2O$	AlF_6	7.5	0.15	−10	[113]
NH_4AlF_4	AlF_6	10	0.1	−6	[113]
$KAlF_4$	AlF_6	12	0.0	−5	[113]
	AlF_6	-	-	−19.5	[114]
K_3AlF_6	AlF_6	-	-	−1.2	[114]
Tl_2AlF_5	AlF_6	-	-	−0.8	[114]
α-$BaAlF_5$	AlF_6	-	-	−13.4	[114]
β-Ba_3AlF_9	3 sites	0.14-0.51	0.07-0.85	−2-1	[115]
$Ba_3Al_2F_{12}$	AlF_6	-	-	−11.7	[114]
β-$CaAlF_5$		1.53	0.10	-	[116]
$RbAlF_4$	AlF_6	13	0.1	−4	[113]
$Al_{13}Si_5O_{20}(OH,F)_{18}Cl$ (zunyite)	$Al1_{Keggin}$	2.25	1.0	72.2	[117]
	$Al1_{Pentamer}$	1.96	0.7	46.5	[117]
	$Al2_{without\ F}$	2.80	0.4	7.8	[117]
	$Al2_{with\ one\ F}$	7.08	0.4	14.0	[117]
$Al_2SiO_4F_2$ (topas)	AlF_6	1.7	0.4	0.3	[113]
Na_3AlF_6 (cryolite)	AlF_6	0.58	0.89	−0.5	[118]
	AlF_6	0.600	0.9	-	[109]
	AlF_6			−0.8	[114]
	AlF_6	2.0	0	1.4	[110]

K_2NaAlF_6 (elpasolite)	AlF_6	1.4	0	0.8	[110]
$Na_5Al_3F_{14}$	AlF_6 1/2	8.2/6.5	0/1	−1/−3	[110]
Na_2MgAlF_7 (weberite)	AlF_6	2.15	0.56	−5.4	[118]
$Na_3Al_2Li_3F_{12}$ (cryolithionite)	AlF_6	1.03	0.09	−0.5	[118]
$Na_5Al_3F_{14}$ (chiolite)	AlF_6	8.0	0.13	−2.5	[118]
	AlF_6 1/2	5.867/8.000	0.0/0.1	-	[109]
$Na_2Ca_3Al_2F_{14}$	AlF_6	0.433	0	−1.6	[119]
α-$NaCaAlF_6$	AlF_6 (i)/(ii)	3.800/2.933	0.25/0.1	−3.4/−2.2	[119]
β-$NaCaAlF_6$	AlF_6 (i)/ (ii)	1.300/0.400	0/0	−3/−3	[119]

Nitrogen containing materials

$AlO_{4-x}N_x$ (AlON) and $(Si, Al)_x(O, N)_{x+1}$ (SiAlON) materials, see [120], for ceramic [121]					
SiAlON	AlO_6	-		2.8	[122]
γ-AlON	AlO_6	-	-	14	[123]
SiAlON	AlO_4	-		59	[122]
γ-AlON	AlO_4	-	-	66	[123]
AlON or Al_2O_3/AlN composite	$AlNO_3$	-	-	96	[123]
AlON or Al_2O_3/AlN composite	AlN_2O_2	-	-	96	[123]
AlON or Al_2O_3/AlN composite	AlN_3O	-	-	106	[123]
AlN	AlN_4	-	-	114-117	[123]
$CaMg_2AlN_3$	AlN_4	5.6	-	120	[124]

Others

Al_4C_3	Al1	15.58	0	120.1	
	Al2	15.38	0	11.2	
$Al(acac)_3$	AlO_6	3.03	0.15	0.0	[125]
$Al(trop)_3$		4.43	0.08	36.6	[125]
$Al(TMHD)_3$	AlO_6	3.23	0.10	1.5	[125]
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	[126]
$NaAlCO_3(OH)_2$ (dawsonite)		6.70	0.45	10	[127]
$Ca_6Al_2S_3H_{64}O_{50}$	AlO_6	0.36	0.19	13.1	[21]
$Ca_4Al_2SH_{24}O_{22}$	AlO_6	1.7	qp	11.8	[21]
$[Al_8(OH)_{14}(H_2O)_{18}](SO_4)_5{\cdot}16H_2O$	3 sites	3.2/5.75/3.1	0.8/0.1/0.5	4.8/8.4/11.0	[128]
$Al_2(OH)_2(H_2O)_8(SO_4)_2{\cdot}2H_2O$	AlO_6	4.6	0.4	3	[3]
$Al_2(OH)_4SO_4{\cdot}7H_2O$ (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	[129]
sample A01 from 6 samples	Al_{I1}/ Al_{I2}	-	-	−3.3/0.1	[129]
$KAl(SO_4)_2{\cdot}12H_2O$	AlO_6	0.400	0.00	−4.1	[27]
$NH_4Al(SO_4)_2{\cdot}12H_2O$	AlO_6	0.456	0.00	−0.4	[27]

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	[130]	
		1.4	0.7	22.1	[131]	
		1.46	0.71	22.65*	[132]	
$Na_2SiO_3{\cdot}9H_2O$		1.110	0.63	3.7	[133]	
$Na_2SiO_2(OH)_2{\cdot}8H_2O$		1.14	0.56	3.53*	[132]	
$Na_2SiO_2(OH)_2{\cdot}4H_2O$	Na 1/2	1.80/2.83	0.75/0.17	9.00*/9.50*	[132]	
α-$Na_2Si_2O_5$		1.820	1	17.1	[130]	
		1.79	1.0	16.9	[134]	
		1.82	1	17.1	[135]	132.3 MHz
$Na_2Si_2O_5$, SKS-5, layered, hydrated, site 2		1.6	0.8	0.8	[136]	
	site 3/4	0.5/1.2	qp/0.2	−1.0/−0.7	[136]	
$Na_2Si_2O_5$, SKS-6, layered, hydrated, site 5/6		1.7/1.6	0.5/0.8	−1.1/0.8	[136]	
	site 7/8	1.2/0.6	0.2/ qp	−1.0/−1.0	[136]	
δ-$Na_2Si_2O_5$	Na_b 5 c	2.4	1	10	[130]	
	site B	2.4	1.0	8.4	[137]	
	(2)	2.4	1	9.1	[135]	132.3 MHz
	Na_c 6 c	1.1	0.3	15.9	[130]	
	site A	1.1	0.3	15.4	[137]	
	(1)	1.16	0.25	16.1	[135]	132.3 MHz
β-$Na_2Si_2O_5$	Na(1)	2.29	0.85	15.6	[134]	
	(2)	2.5	0	18.7	[135]	132.3 MHz
	Na(2)	2.20	0.55	9.4	[134]	
	(1)	2.22	0.55	9.4	[135]	132.3 MHz
$Na_2O{\cdot}4SiO_2{\cdot}5H_2O$ (makatite)	site 1/2/3	1.3/1.5/1.4	0.6/0.4/0.6	0/1/8	[138]	
$Na_2O{\cdot}8SiO_2{\cdot}9H_2O$ (octosilicate)		0.48	-	−0.7	[138]	
$Na_2O{\cdot}8SiO_2{\cdot}xH_2O$ (octosilicate dried)		2.4	0.7	−6	[138]	
$NaSi_2O_5{\cdot}3H_2O$ (kanemite)	site 1/2/3	1.7/2.0/0.6	0.7/0.7/-	0/2/−1	[138]	
$Na_2Si_{14}O_{29}{\cdot}11H_2O$ (magadiite)		1.3	0.6	0	[138]	
$Na_2Si_{22}O_{41}(OH)_8{\cdot}6H_2O$ (kenyaite)		0.60	-	−0.5	[138]	
$Na_8Si_{12}O_{28}{\cdot}4H_2O$ (Mu-11)	(A)/ (B)	2.7/2.9	0.4/0.7	1/0.7	[139]	
$Na_2BaSi_2O_6$	Na 1/Na 2	2.10/2.96	0.75/0.1	25.0/5.4	[134]	
$Na_2H_2SiO_4{\cdot}8H_2O$		1.11	0.72	3.8*	[140]	
$Na_2H_2SiO_4{\cdot}4H_2O$	(1)/(2)	1.80/2.83	0.75/0.17	9.0*/9.5*	[140]	
$10Na_2O$ $10CaO$ $21B_2O_3$ $8Al_2O_3$ $51SiO_2$ (glass)		2.8	0.7	−7.9	[141]	
$43.1Na_2O$ $56.9SiO_2$ (glass)		3.0	-	7.5	[142]	
Soda-lime silicate glass		1.9	-	4.7	[143]	
$Na_4Ti_2Si_8O_{22}{\cdot}5H_2O$ (penkvilksite)		3.30	0.45	4.3	[144]	
Na_3F $SnSi_3O_9$ (stannosilicate)	(A)/ (B)	3.0/3.7	0.55/0.68	12.5/9	[145]	

Aluminosilicates / Zeolites / Sodalites

Na-A (dehydrated) near to 6- rings		5.8	0	-	[146]
near to	4, 8-rings	3.2	0.9	-	[146]
Na-LSX (93.2 Na/u.c.)	SI	1.2	0.1	0	[147]
(dehydrated)	SI'	5.9	0.1	−6	[147]
	SII	5.1	0.2	−12	[147]
	SIII'(1,2)	2.2	0.5	−13	[147]
	SIII'(3)	2.0	0.8	−1	[147]
Na-LSX (dehydrated)	SI	1.1	0.5	5.2*	[148]
	SI'	5.8	0.0	−12.8*	[148]
	SII	5.0	0.0	−8.8*	[148]
	SIII'(1,2)	2.2	0.7	−10.8*	[148]
	SIII'(3)	1.2	0.9	−22.8*	[148]
39Li86NaLSX (dehyd.)	SI	1.1	0.5	5.2*	[148]
	SI'	5.4	0.0	−11.8*	[148]
	SII	4.8	0.1	−8.8*	[148]
	SIII'	0	-	−21.8*	[148]
84Li16NaX (dehydr.)	SIII'	0	-	−22.8*	[148]
Na-X (83.5 Na/u.c.)	SI	1.2	0.1	−1	[147]
(dehydrated)	SI'	5.9	0.1	−10	[147]
	SII	4.8	0.2	−16	[147]
	SIII'(1,2)	2.6	0. 5	−17	[147]
	SIII'(3)	2.0	0.8	−11	[147]
Na-X (Si/Al=1.23) MAS/DOR	SI	0/-	0/-	1.2/-*	[149]
(dehydrated)	SI'(1)	5.2/5.0	0/0	−11.8/−12.8*	[149]
	SI'(2)	-/3.6	-/0	-/−20.8*	[149]
	SII	4.6/4.5	0/0.1	−7.8/−10.8*	[149]
	SIII'(1,2)	2.6/3.0	0.7/0.5	−5.8/−3.8*	[149]
	SIII'(3)	1.6/1.9	0.9/0.9	−21.8/−23.8*	[149]
Zeolite Na-X (Si/Al=1.24)	SI	1.4	0	−2.7	[150]
(dehydrated)	SI'	5.4	0	−20	[150]
	SII	4.9	0	−10	[150]
	SIII'(1,2)	3.0	0.5	−11	[150]
	SIII'(3)	2.1	0.9	−21	[150]
Na-Y (Si/Al=2.5) (dehydrated)	SI	0	0	−4.8*	[149]
Na-Y (Si/Al=2.6) (dehydrated)	SI	1.2	qp	−5	[151]
	SI	1.2	0	−1.5	[150]
	SI'	4.8	0	−12	[150]
	SII	3.9	0	−8	[150]
Na-Y (Si/Al=2.7) (dehydrated)	SI	1.2	$0.5_{assumed}$	−3.3*	[152]
	SI'	2.6	$0.5_{assumed}$	−5.4*	[152]
	SII	3.8	$0.5_{assumed}$	−13.0*	[152]
Na-Y (Si/Al=8.6) (dehydrated)	two SI sites	1.1/1.2	$0.5_{assumed}$	−1.2/−6.1*	[152]
	in sodalite c.	1.6	$0.5_{assumed}$	−18.1*	[152]
	SII	3.5	$0.5_{assumed}$	−11.7*	[152]
Na-Y (Si/Al=2.56) (dehydrated)	SI	0.4	qp	−6	[153]
	SI'/SII'	2.3	qp	−12	[153]
	SII	4.2	qp	−4	[153]
	SIII	4.7	qp	5	[153]
Na-Y (Si/Al=2.6) (dehydrated)	SI	1.2	0.1	−3	[147]
	SI'	4.8	0.2	5	[147]
	SII	3.9	0.2	−7	[147]

HNa-Y (21.3 Na/u.c.) (dehyd.)	SI	1.2	0.1	−3	[147]
	SI’	4.9	0.2	5	[147]
	SII	3.8	0.2	−7	[147]
HNa-Y (13.3 Na/u.c.) (dehydr.)	SI	1.2	0.1	−3	[147]
	SI’	4.9	0.3	5	[147]
	SII	3.8	0.2	−7	[147]
HNa-Y (2.7 Na/u.c.) (dehydr.)	SI	1.2	0.1	−3	[147]
	SI’	4.8	0	3.2*	[149]
	SII	3.9	0	−4.8*	[149]
$Ca_{19}Na_{16}$-Y (Si/Al=2.56) (dehy.)	SI	0.4	qp	−2	[153]
	SI’/SII’	2.3	qp	−4	[153]
	SII	4.6	qp	−3	[153]
	SIII	5.0	qp	3	[153]
75Na25K chabazite (dehydr.)	SIIa	5.7	qp	−8.1*	[154]
	SIII'a	4.1	qp	−17.5*	[154]
	SIII’b	1.7	qp	−2.8 to −15.6*	[154]
31Li47Na22K chabazite (dehy.)	SI	1.2	qp	6.2*	[154]
	SIIa	4.9	qp	−6.8*	[154]
	SIIb	5.3	qp	−4.8*	[154]
	SIII'a	4.1	qp	−17.8*	[154]
	SIII’b	2.0	qp	−3.8 to −13.1*	[154]
64Li13Na23K chabazite (dehy.)	SIII'a	4.4	qp	−15.8*	[154]
Na-EMT (Si/Al=3.7) (dehydr.)	SI	1.0	qp	−6.5	[151]
Na-MOR (Si/Al=7.1) (dehydr.)	12-ring	2.0	qp	−14	[151]
	sidepockets	3.1	qp	−24	[151]
Na-ZSM-5 (Si/Al=18) (dehydr.)	10-ring	2.0	qp	−18	[151]
$Na_2Al_2Si_3O_{10}\cdot 2H_2O$ (natrolite)		1.82	0.6	8.18	[155]
$NaAlSi_3O_8$ (albite)		2.69	0.25	−7.1	[156]
$NaAlSi_2O_6$		3.3	0.25	11.0	[134]
Na,K $AlSi_3O_8$ (feldspar)	8 samples	2.136-1.160	0.6-0.7	−20.1-−24.7	[61]
$Na_8Al_2Be_2Si_8O_{24}Cl_2$ (tugtupide)		1.41	0.44	7.7	[58]
$Na(Na_2)Mg_5Si_8O_{22}(OH)_2OH$	M(4)	3.9	0.49	9.3	[63]
(HSMC)	channel (A)	2.9	0.26	5.5	[63]
$Na_{8.0}[AlSiO_4]_6Cl_{1.8}\cdot 0.4\ H_2O$ (NaCl-sodalite)		0.20-0.45	qp	−8.8	[66]
$Na_{7.7}[AlSiO_4]_6Br_{1.8}\cdot 0.4\ H_2O$ (NaBr-sodalite)		0.72	0.12	−9.9	[66]
$Na_{7.8}[AlSiO_4]_6I_{1.7}\cdot 0.4\ H_2O$ (NaI-sodalite)		1.73	0.06	−20.6	[66]
$Na_8Cl_2[Al_6Si_6O_{12}]$ (NaCl-sodalite)		≈0	$0.67_{assumed}$	6.3	[157]
$Na_8B_2[Al_6Si_6O_{12}]$ (NaB-sodalite)		1	$0.67_{assumed}$	8.5	[157]
$Na_8I_2[Al_6Si_6O_{12}]$ (NaI-sodalite)		1.9	$0.67_{assumed}$	9.3	[157]
$Na_8Cl_2[Al_6Si_6O_{24}]$ (NaCl-sodalite)		0.5	qp	6.1	[64]
$Na_8Br_2[Al_6Si_6O_{24}]$ (NaBr-sodalite)		0.7	qp	7.2	[64]
$Na_8I_2[Al_6Si_6O_{24}]$ (NaI-sodalite)		1.8	qp	7.3	[64]
$Na_8[Al_6Si_6O_{24}]\cdot(H_3O_2)_2$ (basic sodalite)		0.8	qp	5	[67]
$Na_8Br_2\ [Al_6Si_6O_{24}]\cdot$ (basic sodalite)		0.7	qp	7.5	[67]
$Na_6[Al_6Si_6O_{24}]\cdot(4H_2O)_2$ (hydro sodalite)		1.1	qp	−0.1	[67]
$Na_8Br_2\ [Al_6Si_6O_{24}]$		0.7	qp	7.4	[67]
$Na_6[Al_6Si_6O_{24}]$ (dry sodalite)		5.6	qp	-	[67]
$Na_8Br_2\ [Al_6Si_6O_{24}]$ (dry sodalite)		0.7	qp	7.4	[67]
$Na_6[AlSiO_4]_6$ (anhydrous sodium sodalite)		5.90	0.10	10.2*	[132]
$Na_8[AlSiO_4]_6(OH)_2$ (hydroxosodalite, dehyd.)		2.00	0.10	3.2*	[132]
$Na_8[AlSiO_4]_6(OH)_2\cdot 2H_2O$ (hydroxosodalite)		1.55	0.16	−1.2*	[132]
Na-nitride sodalite		1.00	0.18	0.4*	[140]

$Na_8Cl_2(AlSiO_4)_6$ (blue sodalite)		0.081	0.35	95 ?	[65]
$Na_8Si_{12}O_{28}\cdot 4H_2O$ (Mu-11)	(A)	2.7	0.4	1	[139]
	(B)	2.9	0.7	0.7	[139]
$Na_6Zn_2[AlSiO_4]_6(SO_4)_2$		1.9	qp	1	[69]
$NaAlSi_2O_6$ (jadeite)		3.30	0.25	11.0	[134]
$(Na_4BH_4)^{3+}$ sodalite	AlSi	8.82	0	−6.61	[158]
	GaSi	6.41	0	−1.31	[158]
	AlGe	6.75	0.22	−1.60	[158]
Al_2O_3-B_2O_3-SiO_2-Na_2O glasses		2.5-3.5	qp	−3-−12	[81]
Soda-lime aluminosilicate glass		1.8	-	−6.9	[143]
$[Na_2O\cdot Li_2O]_{0.46}[0.16Al_2O_3\cdot 0.84P_2O_5]_{0.54}$ glass					
	$Al(OP)_6$	2.4-2.6	qp	−10-−11	[159]
	$Al(OP)_5$	3.3-4.0	qp	16-18	[159]
	$Al(OP)_4$	3.4-4.2	qp	46-49	[159]
Nitrogen containing materials					
$NaNO_3$		-	-	−7.3	[160]
		0.337	0.00	−8.0	[27]
$NaNO_2$		1.09	0.11	−0.1	[27]
NaN_3		-	-	−3.5	[160]
		0.297	0.12	−3.8	[27]
Phosphorus containing materials					
$Na_3P_3O_9$	Na 1/Na 2	2.20/1.57	0.70/0.55	−7.60*/1.60*	[132]
$Na_5P_3O_{10}\ H_2O$	1/2	1.74/1.97	0.29/0.85	−0.55/−5.71	[161]
	3/4	2.09/2.40	0.81/0.51	−9.09/2.20	[161]
	5	1.69	0.26	−4.20	[161]
$Na_5P_3O_{10}$	Na 1/ Na 2	4.65/3.06	0.40/0.17		[162]
	Na 3	4.65	0.40		[162]
$Na_2P_2O_7\ H_2O$	Na 1/ Na 2	1.37/0.48	0.92/0.99	-	[162]
$Na_4P_2O_7$	Na 1/ Na 2	2.08/2.30	0.26/0.70	5.52/1.96	[163]
	Na 3/ Na 4	2.90/3.22	0.47/0.56	10.41/6.36	[163]
$Na_4P_2O_7\ 10H_2O$		-	-	1.5	[160]
$Na_3HP_2O_7\ H_2O$	Na 1/ Na 2	2.55/3.60	0.15/0.20	4.0/1.0	[163]
	Na 3	3.1	0.1	6.5	[163]
Na_2HPO_4	Na 1/ Na 2	0.210/0.325	0.18/0.7	−1.4/−2.5	[164]
	Na 3	0.589	0.26	−1.1	[164]
$NaH_2PO_4\cdot 2H_2O$		1.19	0.46	2.40*	[132]
$NaH_2PO_4\cdot H_2O$		1.22	0.26	−3.49*	[132]
NaH_2PO_4	Na 1/ Na 2	1.59/2.35	0.46/0.94	-	[162]
$CaNa_4(P_3O_9)_2$	50%/50%	1.405/2.191	0.60/0.69	−3.3/−13.3	[165]
$NaMg(PO_3)_3$	43%/26%	2.67/2.57	0.34/0.47	0.0/−4.3	[166]
	31%	2.72	0.59	−9.8	[166]
$NaZn(PO_3)_3$	41%/28%	2.50/2.66	0.38/0.51	0.0/−4.1	[166]
	31%	2.67	0.59	−9.9	[166]
$NaCa(PO_3)_3$	93%/7%	2.15/0.62	0.88/0.99	3.73/−5.58	[167]
$NaSr(PO_3)_3$		2.38	0.70	2.74	[167]
$NaPO_3$ glass		2.1	qp	−3.4	[168]
$NaPO_3$ glass		2.52	qp	−5.1	[169]
$Na_{0.2}Li_{0.8}PO_3$ glass		2.65	qp	−7.0	[169]
$Na_{0.2}Ag_{0.8}PO_3$ glass		2.41	qp	−5.5	[169]
$Na_{0.22}K_{0.78}PO_3$ glass		2.34	qp	−1.0	[169]

$Na_{0.22}Rb_{0.78}PO_3$ glass		1.93	qp	−0.6	[169]
$Na_{0.19}Cs_{0.81}PO_3$ glass		2.52	qp	−1.7	[169]
$Na_{0.2}Li_{0.8}PO_3$ glass		2.65	qp	−7.0	[169]
$NaPO_3$ −WO_3 glass		2.0	qp	−14.9	[168]
$NaPO_3$− GeO_2 glass		1.8	qp	−4.5	[170]
$(M_2O)_{1/3}[(Ge_2O4)_x(P_2O_5)_{1-x}]_{2/3}$ glass M = Na, K x = 0.0, 0.4, 0.8		1.3/1.7/1.6	qp	−5.7/−8.3/−4.0	[171]
$60NaPO_3$−$40MoO_3$ glass		2.0	qp	−14.3	[172]
$Na_{1.4}Al_{0.4}Ti_{1.6}(PO_4)_3$		1.4614	-	−8.3	[173]
$Na_{1.4}Al_{0.4}Zr_{1.6}(PO_4)_3$		1.1200	-	−14.6	[173]
$Ca_{10}K_{0.5}Na_{0.5}(PO_4)_7$		2.4	0.13	−8.8	[174]
$NaSn_2(PO_4)_3$	Na 1/Na 2	2.3/2.5	0/0	-	[175]
$Na_3Fe_3(PO_4)_4$ (layered)	Na 1/Na 2	1.55/1.57	0.03/0.48	277.5/143.0	[176]
$[Na_2O{\cdot}Li_2O]_{0.46}[0.16Al_2O_3{\cdot}0.84P_2O_5]_{0.54}$ glass		1.3	qp	−6	[159]
$Ca_{10}K_{0.5}Na_{0.5}(PO_4)_7$		2.4	0.13	−8.8	[174]
$Ca_{10}Na(PO_4)_7$		2.48	0.2	−5	[177]
$Na_3MnPO_4CO_3$ (sidorenkite)	1/2	1.2/4.4	0.0/0.5	−168/569	[178]
$Na_6[P_2Mo_5O_{23}]{\cdot}7H_2O$	Na(a)/ Na(d)	3.15/2.49	qp/ qp	−1.6/−11.0	[179]
	Na(f)	0.88	qp	−2.1	[179]
HNaPW (hydrated)	1/2	2.0/2.7	1.0/0.0	3/4	[180]
$Na_{15}[(PO_2)_3PNb_9O_{34}]{\cdot}22H_2O$	5 sites	0.63-2.2	0-1	−8.4-3.1	[181]
$Na_5B_2P_3O_{13}$	5 sites	1.54-2.83	0.02-0.85	−7.7-9.2	[182]
Others					
Na_4Si_4 (2 at% P-doped)	Na-Si	1.25	1.0	56.7	[183]
	Na-Si	2.31	0.15	49.5	[183]
	Na-P	2.0	0.1	53.3	[183]
Cs_7NaSi_8		5.36	0	72.2	[184]
Rb_7NaSi_8		5.66	0	157.2	[184]
Na_2O		≈0	-	55.1	[185]
Na_2O_2	2 sites	-	-	4.8 and 9.9	[186]
Na_3OCl		11.34	0.0	-	[185]
NaOH	5-coord.	3.59	0.07	21.1	[187]
		3.5	0.00	19.4*	[132]
$NaOH{\cdot}2H_2O$		2.20	0.70	12.2*	[132]
$NaZrO_3$	Na 1/ Na 2	2.52/2.08	0.67/0.05	15.0/27.0	[188]
	Na 3	4.20	0.27	19.5	[188]
$Na_2ZrSi_2O_7$ (parakeldyshite)	Na 1/Na 2	1.5/2.8	1.0/0.85	0.0/2.0	[189]
$Na_2ZrSi_4O_{11}$ (vlasovite)	Na 1/Na 2	1.65/4.70	0.25/0.0	−4.5/−3.0	[189]
$NaZrSi_6O_{15}{\cdot}3H_2O$ (elpidite)	Na 1/Na 2	2.05/2.65	0.50/0.75	−7.0/−1.0	[189]
$Na_4Zr_2Si_3O_{12}$	Na 1/Na 2	2.30/3.10	0.85/0.30	−7.0/9.0	[189]
NaF		-	-	7.9	[160]
	octahedr.	≈0	-	7.2	[187]
NaCl		-	-	7.9	[160]
	octahedr.	≈0	-	7.2	[187]
NaBr		-	-	6.0	[160]
	octahedr.	≈0	-	5.1	[187]
NaI				−2.7	[160]
	octahedr.	≈0	-	−3.2	[187]
$NaIO_4$		-	-	−12.5	[160]
Na_2S	tedrahedr.	≈0	-	49.7	[187]
α-$NaVO_3$	Na 1/ Na 2	1.5/0.765	0.58/0.06	−15.5/−4.8	[190]

β-$NaVO_3$		1.42	0.27	−10.3	[190]	
Na_2SO_4		2.60	0.58	−1.3*	[132]	
Na_2SO_3	Na 1/ Na 2	1.06/0.33	0.00/0.00	-	[162]	
	Na 3	1.14	0.00	-	[162]	
$NaAlO_2$		2.15	0.60	26.2*	[132]	
$Na[Al(OH)_4]$		3.10	0.00	5.9	[191]	
$NaAl_9O_{14}$	1/2	2.15/2.65	0.4/0.2	−15.6/−14.6	[28]	
$Na_2Al_2B_2O$	Na 1/Na 2	1.9/0.33	0.1/0	5.5/−7.1	[105]	
Na_2B_{29}	50%/50%	2.4/2.2	qp/ qp	10.2/16.9	[192]	
$NaBO_2$		1.19	0.24	2.1	[106]	
		1.2	0.09	1.8	[193]	
$Na_4B_2O_5$	Na 1/Na 2	2.2/3.0	1.0/0.5	19.6/14.4	[193]	
$Na_2O{\cdot}4B_2O_3$	Na 1/Na 2	4.1/2.0	0.18/0.35	3.4/ −11.4	[193]	
$NaBO_2{\cdot}2H_2O$		1.530	0.80	10.6	[133]	
$Na_2B_4O_7$	62%/20%	2.65/1.8	0.91/0.9	−9.9/−12.0	[106]	
	18%	1.8	0.1	−4.9	[106]	
$Na_2B_4O_7{\cdot}10H_2O$ (borax)	Na 1/Na 2	0.541/0.849	0.499/0.143	-	[194]	
$Na_2B_4O_7{\cdot}5H_2O$ (tincalconite)	Na 1/Na 2	0.539/0.785	0.741/0.0	-	[194]	
	Na 3	1.299	0.0	-	[194]	
$NaCa[B_5O_6(OH)_6]{\cdot}5H_2O$ (ulexite)		0.07	-	7.1	[195]	
$NaSnO_3{\cdot}3H_2O$		1.760	0.00	12.8	[133]	
$NaTeO_4{\cdot}2H_2O$		2.240	0.37	12.5	[133]	
$Na_2Te_4O_9$	Na 5/Na6	4.4/3.6	0.08/0.12	−3/5	[196]	
Na_2TeO_3	Na 1/Na2	1.84/1.36	0.08/0-12	5.8/17.0	[196]	
$NaNbO_3$ (polar phase)	Na 1/ Na 2	2.4/1.2	qp/ qp	1.5/−5.1	[197]	
$NaNbO_3$ (perovskite)		1.3	0.9	−3.0	[198]	MAS
$Li_{0.05}Na_{0.95}NbO_3$	Na 1/ Na 2	1.1/2.3	qp/ qp	−4.6/−0.6	[199]	
$NaNbWO_6$	19%/81%	0.4/1.4	0.5/-	−6.5/−18	[200]	
$NaTaO_3$ (perovskite)	Na 1/Na 2	2.1/1.0	0.0/0.9	−0.5/−4.5	[198]	
Na_2CrO_4	Na 1/Na 2	2.78/0.5	0.57/ qp	−12.8*/−6.7*	[132]	
$NaClO_4$		-	-	−20.4	[160]	
		0.80	0.35	−18.3*	[132]	
$NaClO_4{\cdot}H_2O$	Na 1/Na 2	1.71/1.48	0.20/0.10	−4.5*/−5.2*	[132]	
$Na_{1-x}Ge_{3+z}$ ($Na_{0.72}Ge_{3.13}$)	Na6	-	-	20.5	[201]	
	Na5(1)/(2)	0.473/0.414	0.25/0.23	4.5/2.4	[201]	
$Na_2Ge_2O_5$		2.3	1.0	14.5	[202]	
$32Na_2O{\cdot}68GeO_2$ (glass)		3.2	qp	7.9	[202]	
$14Na_2O{\cdot}86GeO_2$ (glass)		2.5	qp	−4.1	[203]	
Na_2GeO_3		1.3	0.8	22.6	[193]	
$Na_4Ge_9O_{20}$		2.7	0.54	−2.1	[193]	
$Na_2Ge_4O_9$		2.4	0.7	−6.4	[193]	
Na_2MoO_4		2.59	0.00	3.2	[204]	
$Na_2MoO_4{\cdot}2H_2O$	Na(1) octah.	0.875	0.23	−1.4	[204]	
	Na(2) trig.	2.68	0.08	4.0	[204]	
$60NaPO_3$-$40MoO_3$ (glass)		2.0	qp	−14.3	[172]	
Na_3UO_4	site A/B/C	3.4/4.0/2.5	qp	47/18/13	[205]	
	site D/E/F	2.6/2.2/2.4	qp	2/−2/−16	[205]	
$NaUO_3$		1.7	0.5	−29.2	[206]	
Na_4UO_5		3.2	0.2	15.1	[206]	
$Na_2U_2O_7$	1/2	1.4/2.0	qp/ qp	−19/−14.1	[206]	
Na_2WO_4		2.49	0.00	4.5	[204]	
$Na_2WO_4{\cdot}2H_2O$	Na(1) octah.	0.88	0.35	−0.9	[204]	

	Na(2) trig.	2.7	0.09	6.3	[204]
Na_2WO_4	(A)	5.2	0.0	−4.0	[207]
	(B)/(C)	small/ small	-	−6/−14	[207]
$[Na_2S]_{2/3}[(B_2S_3)_{1/2}(P_2S_5)_{1/2}]_{1/3}$ (glass)		1.6	qp	3.8	[208]
Na_3AlF_6 (cryolite)	CN 6	0.83	0.62	2.6	[118]
	Na1	0.840	0.6	2	[109]
	CN 8 site 1	1.43	0.27	−8.4	[118]
	Na2	1.430	0.3	−9	[109]
$Na_5Al_3F_{14}$ (chiolite)	Na1/ Na2	1.480/3.180	0.0/0.1	−24/−9	[109]
Na_2MgAlF_7 (weberite)	CN 8 site 1/2	2.48/3.24	0.08/0.26	−28.6/−10.4	[118]
$Na_2Ca_3Al_2F_{14}$		3.360	0	5.2	[119]
α-$NaCaAlF_6$	(i)/ (ii)	2.340/1.360	0.25/0.1	2.0/−1.6	[119]
β-$NaCaAlF_6$		1.200	1	7	[119]
$NaCoO_2$		3.98	0.02	48	[209]
Na_3AlH_6 doped/non-doped site	Na1	0.50/0.49	0.6/0.7	23.5/23.3	[40]
Na_3AlH_6 doped/non-doped site	Na2	0.93/0.93	0.4/0.4	−8.8/−8.9	[40]
Na_2LiAlH_6		<0.1	-	−17.9	[40]
$NaAlH_4$		0.15	0.2	−9.2	[40]
NaH		<0.1	-	18.2	[40]
$NaHCO_3$				−5.4	[160]
$NaAlCO_3(OH)_2$ (dawsonite)		3.64	0.56	2	[127]
$Na_2C_2O_4$		2.43	0.75	-	[162]
Na_3C_{60}		3.3	0.08	17.2	[210]

Table 8.3. ^{17}O, quadrupole coupling constant $C_\mathrm{Q} = e^2qQ/h$, 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 [211]. Reviews concerning solid-state ^{17}O NMR investigations of inorganic material were presented by Asbrook and Smith [212, 213], Gerothanassis [214], and MacKenzie and Smith [120]. The data in the table, which were published in the years 1989-2000, were compiled by Pingel [215]. 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 $P_\mathrm{Q} = C_\mathrm{Q}\sqrt{1+\frac{\eta^2}{3}}$ instead of C_Q.

Compound	site	C_Q/ MHz	η	δ /ppm	Refs.
Aluminum hydroxides, aluminates					
AlO(OH) (boehmite)	OAl_4	1.20	0.1	70	[216]
	OAl_4	1.15	0.13	70.0	[27]
	Al_2OH	5.0	0.5	40	[216]
$Al(OH)_3$ (bayerite)	Al_2OH	6.0	0.3	40	[216]
α-Al_2O_3 (corundum)	OAl_4	2.17	0.55	75	[216]
	OAl_4	2.13	0.50	72	[10]
	OAl_4	< 2.4	-	66	[217]
γ-Al_2O_3	OAl_4	1.8	qp	73	[216]
η-Al_2O_3	OAl_4	1.6	qp	73	[216]
δ-Al_2O_3	OAl_4	1.6	qp	72	[216]
θ-Al_2O_3	OAl_4	1.2	qp	72	[216]
	OAl_3	4.0	0.6	79	[216]
$Al_{13}O_{40}$ cluster	AlOAl	1.2	0	50	[218]
$NaAlO_2$	AlOAl	1.81	qp	30.9	[219]
$CaAl_2O_4$	nb O	≈1.9	qp	≈141	[219]
	8 br O	1.3-1.9	qp	57.3-86.8	[220]
$CaAl_4O_7$	O1	1.9	0.7	71.6	[220]
	O2 or O3	1.8	0.5	61.5	[220]
	O3 or O2	2.1	0.5	56.8	[220]
	O4	2.5	0.4	40.6	[220]
$LaAlO_3$		1.6 (max.)		170.2	[221]
$Y_3Al_5O_{12}$	OY_2Al_2	1.49	0.99	142	[10]
$Y_4Al_2O_9$	9 sites	1.49	qp	126-372	[10]
$YAlO_3$	$O_{(1)}Y_3Al_2$	1.57	1.00	143	[10]
	$O_{(2)}Y_3Al_2$	1.65	0.35	165	[10]
Silicates without aluminum					
Siliceous zeolite Y, Sil-Y	SiOSi O1	5.1	0.3	42.3	[222]
dehydrated	SiOSi O2	5.39	0.2	37.2	[222]
	SiOSi O3	5.14	0.1	47.3	[222]
	SiOSi O4	5.28	0.2	34.8	[222]
Siliceous ferrierite, Sil-FER	SiOSi 1	5.62	qp	43.1	[223]
dehydrated	SiOSi 2	5.22	qp	41.6	[223]
	SiOSi 3	5.35	qp	40.7	[223]
	SiOSi 4	5.29	qp	39.6	[223]
	SiOSi 5	5.38	qp	39.0	[223]
	SiOSi 6	5.27	qp	37.0	[223]
	SiOSi 7	5.32	qp	37.0	[223]
	SiOSi 8	5.46	qp	35.9	[223]
	SiOSi 9	5.64	qp	34.8	[223]

	SiOSi 10	5.57	qp	28.0	[223]
SiO_2 (low cristobalite)	SiOSi	5.3	0.0	44	[224] MAS
SiO_2 (α-cristobalite)	SiOSi	5.3	0.125	36.7	[225]
		5.35	0.21	37.5	[226]
SiO_2 (α-quartz)	SiOSi	5.21	0.19	43	[226]
SiO_2 (amorphous)	SiOSi	5.8	0.0	50	[227]
	SiOH	4.0	0.3	20	[227]
	SiOH	4.4	0.0	37	[228]
SiO_2 (stishovite)	OSi_3	6.5	0.125	109	[229]
SiO_2 (coesite)	SiOSi O5	5.16	0.292	58	[230]
	SiOSi O2	5.43	0.166	41	[230]
	SiOSi O3	5.45	0.168	57	[230]
	SiOSi O4	5.52	0.169	53	[230]
	SiOSi O1	6.05	0.000	29	[230]
SiO_2 (glass)	SiOSi	5.08	0.150	37.58	[231]
$2Mg_2SiO_4{\cdot}Mg(OH)_2$ (hydr.-chondrodite)	OH	6.6	0.1	25	[232]
$4Mg_2SiO_4{\cdot}Mg(OH)_2$ (hydr.-clinohumite)	OH	7.0	0.2	25	[232]
β-Mg_2SiO_4 (hydr. wadsleyite)	O2	4.9	0.9	76	[233]
		5.0	0.9	78	[234]
	O3	4.4	0.2	66	[233]
	O4	3.8	0.3	65	[233]
	O1	1.3	qp	38	[233]
Mg_2SiO_4 (forsterite)	SiOMg-I	2.35	0.2	61	[235]
		2.8	qp	64	[236]
	O3	2.5	0.2	61	[237] 3QMAS
	SiOMg-II	2.35	1.0	62	[235]
		3.3	qp	72	[236]
	O2	2.5	0.4	64	[237] 3QMAS
	SiOMg-III	2.70	0.3	47	[235]
		3.0	qp	49	[236]
	O1	2.9	0.3	48	[237] 3QMAS
$Mg_3Si_4O_{10}(OH)_2$ (talc)	SiOMg	3.2	0.0	40	[227]
	SiOSi	5.8	0.0	50	[227]
	MgOH	7.3	0.0	0	[227]
$2Mg_2SiO_4{\cdot}Mg(OH)_2$ (chondrodite)	O1/O2	2.5/2.3	0.3/0.2	63/60	[232] 3QMAS
	O3/ O4	2.3/2.7	0.3/0.2	59/52	[232] 3QMAS
$4Mg_2SiO_4{\cdot}Mg(OH)_2$ (clinohumite)	O2/ O6	2.5/2.4	0.3/0.2	65/64	[232] 3QMAS
	O3+O4	2.3	0.1	61	[232] 3QMAS
	O7/ O8	2.4/2.4	0.2/0.2	60/59	[232] 3QMAS
	O5/O1	2.7/2.7	0.2/0.2	52/49	[232] 3QMAS
$MgSiO_3$ (ortoenstatite)	O21/ O22	2.8/2.9	qp/ qp	42/46	[238]
	O11/O12	3.0/3.0	qp/ qp	52/54	[238]
	O31/ O32	4.3/4.9	qp/ qp	64/73	[238]
$MgSiO_3$ (protoenstatite)	O1+impurity	2.8	qp	52	[238]
	O2/ O3	2.7/4.3	qp/ qp	39/66	[238]
$MgSiO_3$ (clinoenstatite)	O21/ O22	2.8/2.8	qp/ qp	45/41	[238]
	O11/ O12	3.0/3.0	qp/ qp	51/54	[238]
	O31/ O32	4.3/4.8	qp/ qp	64/75	[238]
	6 sites	2.9–5.2	qp	57-70	[236]
	SiOMg-I	3.2	0.0	60	[239]
	SiOMg-II	3.2	0.0	42	[239]
	SiOSi	5.1	0.3	62	[239]
$Mg_3Si_4O_{10}(OH)_2$ (talc)	SiOMg	3.2	0.0	40	[227]

	SiOSi	5.8	0.0	50	[227]
	MgOH	7.3	0.0	0	[227]
$CaMgSi_2O_6$ (diopside)	SiOCa	2.7	0.0	84	[239]
	SiOCa	2.83	0.13	86	[236]
	O1	2.7	qp	85	[238] 81.4 MHz
	SiOMg	2.7	0.1	63	[239]
	SiOMg	2.74	0.00	64	[236]
	O2	2.9	qp	63	[238] 81.4 MHz
	SiOSi	4.4	0.3	69	[239]
	SiOSi	4.39	0.36	69	[236]
	O3	4.3	qp	70	[238] 81.4 MHz
α-$CaSiO_3$ (pseudowollastonite)	br O	3.8	0.2	75	[239]
	2 nb O	2.3/2.1	0.1/0.1	91/94	[239]
$CaSiO_3$ (wollastonite)	9 sites	2.0-4.8	qp	67-115	[236]
Ca_2SiO_4 (larnite)	4 sites	2.5-2.9	qp	122-134	[236]
$38.5CaO{\cdot}61.5SiO_2$ (glass CS46)	nb O	2.1	qp	104.7	[240]
	SiOSi	4.3	qp	62.7	[240]
$Li_2Si_2O_5$	br O1	5.6	0.55	108	[241]
	br O2	4.05	0.05	35	[241]
	nb O3	2.45	0.1	38	[241]
$Li_2Si_2O_5$ (glass)	br O	5.0	0.15	68	[241]
	nb O	2.55	0.2	42	[241]
Na_2SiO_3	br O2	4.20	0.58	63	[131]
	nb O1	2.43	0.17	39	[131]
α-$Na_2Si_2O_5$	br O1	5.74	0.2	52	[241]
		5.7	0.0	55	[229]
	br O2	4.67	0.3	74	[241]
		4.7	0.25	55	[229]
	nb O3	2.4	0.2	36	[241]
		2.35	0.1	34	[229]
ϵ-$Na_2Si_2O_5$	nb O	-	-	45	[229]
$Na_2Si_2O_5$ (glass)	br O	4.9	0.1	69	[241]
	nb O	2.35	0.2	37	[241]
$Na_2Si_4O_9$ (glass)	SiOSi	5.2	0.22	51	[242]
	nb O	2.7	0.25	40	[242]
	H_2O	6.0	0.7	20	[242]
$Na_2Si_3O_7$ (glass)	br O	5.0	0	60	[229]
	nb O	2.3	0	39	[229]
$24Na_2O{\cdot}76SiO_2$ (glass)	SiOSi	4.73	0.5	48.3	[243]
	SiONa	2.03	0.6	32.2	[243]
$Na_8Si_{32}O_{64}(OH){\cdot}32H_2O$	SiOSi	5.1	0	42.6	[244]
(sodium ilerite, RUB-18)	SiOH	3.1	0	61.2	[244]
$Na_4Zr_2Si_3O_{12}$	SiOZr 1	2.68	0.0	169.5	[189]
	SiOZr 2	2.75	0.1	118.0	[189]
	SiOZr 3	2.80	0.2	126.0	[189]
$ZrSiO_4$	SiOZr	-	-	160	[189]
$K_2Si_2O_5$	br O1	5.1	0.1	114	[241]
	br O2	4.7	0.2	69	[241]
	nb O3	2.1	0.5	72	[241]
$K_2Si_2O_5$ (glass)	br O	4.7	0.25	60	[241]
	nb O	2.5	0.45	84	[241]
$K_2Si_4O_9$ (wadeite)	br O1	4.45	0.35	62.5	[229]
	SiOSi O2	4.90	0.2	97	[229]

$KHSi_2O_5$	br O	4.9	0.1	51	[245]
	nb O	3.5	0.35	60	[245]
$K_2Si_4O_9$ (glass)	br O	4.9	0	52	[229]
	nb O	2.3	0	76	[229]
$Rb_2Si_2O_5$	br O1	4.4	0.1	124	[241]
	br O2	4.7	0.5	59	[241]
	nb O3	1.9	0.5	93	[241]
$Cs_2Si_2O_5$ (glass)	br O	4.55	0.3	68	[241]
	nb O	3.1	0.55	145	[241]
$BaSiO_3$	br O	3.7	0.4	87	[239]
	nb O	1.6	0.1	159	[239]
	nb O	2.1	0.1	169	[239]
$Ba_2TiSi_2O_8$ (fresnoite)	SiOTi	-	-	190 (anisotr.)	[246]
	SiOSi	3		0 (anisotr.)	[246]
$LiTiOSiO_4$	TiOSi	3.05	0.35	157	[247]
	nb apical OTi	≈0	-	741	[247]
α-$SrSiO_3$	br O	4.1	0.4	80	[239]
	nb O	2.2	0.1	105	[239]
	nb O	2.1	0.1	108	[239]
$La_{9.33}(SiO_4)_6O_2$ (apatite-type)	O1 or O2	0.266	0.6	165	[248]
	O2 or O1	0.305	0.6	214	[248]
	O3	0.264	0.6	194	[248]
	O4	-	-	600	[248]
Soda-lime borosilicate glass	SiOSi	4.91	0.34	48.1	[243]
	SiOB	5.24	0.45	61.9	[243]
	BOB	5.07	0.46	84.3	[243]
	SiONa	2.60	1	35.2	[243]
	SiO(Ca, Na)	4.91	0.89	70.5	[243]
Cesium borosilicate glass,	br O slice 1	qp=4.2	0.6	52.9	[249]
CBS-2-1.5	br O slice 2	qp=4.5	0.3	60.1	[249]
	br O slice 3	qp=4.5	0.3	67.8	[249]
	br O slice 4	qp=4.5	0.6	77.5	[249]
	nb O site 2	qp=2.3	-	123.7	[249]
Cesium borosilicate glass,	SiOSi	qp=5.1	0.4	44.7	[249]
CBS-2-1.5	SiOB	qp=5.6	0.8	67.6	[249]
	BOB	qp=5.4	0.7	98.5	[249]
Sodium borosilicate glass,					
NBS-K0.5R0.25	SiOSi	5.13	qp	42.3	[250]
NBS-K2R0.5	SiOSi	5.08	qp	43.9	[250]
NBS-K4.5R0.75	SiOSi	5.08	qp	44.2	[250]
Barium borosilicate glass	nb BaOSi	2.3	qp	158	[251]
40BaO $30B_2O_3$ $30SiO_2$	nb BaOB	3.6	qp	197	[251]
Ba Si glass	br O	4.0	0.3	78	[252]
Ba Ca Si glass	br O	4.1	0.3	68	[252]
Ca Si glass	br O	4.7	0.3	59	[252]
	br O	4.6	0.0	66	[228]
	nb O	2.1	0.2	110	[228]
$CaTiSiO_5$ (crystalline titanite)	Ti-O-Ti	0.2	≈1	632	[253]
	Si-O-Ti	2.7−3.2	0.1−0.2	166−189	[253]
PbO-SiO_2 glasses	Si-O-Si	4.4-4.1	$0.5_{assumed}$	74.6-80.2	[254]
$0.60 \leq X_{PbO} \leq 0.71$	Pb-O-Si	2.9	$0.5_{assumed}$	150.7-151.7	[254]
	Pb-O-Pb	3.1-3.0	$0.5_{assumed}$	287.5-282.6	[254]

Aluminosilicates and sodalites

Na-A, dehydrated	SiOAl	3.2	0.2	32	[224] MAS
	SiOAl O1	3.5	qp	43.6	[255] 5QMAS
	SiOAl O2	3.6	qp	31.2	[255] 5QMAS
	SiOAl O3	3.4	qp	40.8	[255] 5QMAS
Na-A, hydrated	SiOAl O1	3.4	0	43.6	[256]
	SiOAl O2	3.4	0	31.0	[256]
	SiOAl O3	3.4	0.25	40.5	[256]
	SiOAl O1	3.4	qp	40.9	[257]
	SiOAl O2	3.6	qp	31.7	[257]
	SiOAl O3	3.4	qp	42.4	[257]
	SiOAl O1	3.5	qp	44	[258] 5QMAS
	SiOAl O2	3.6	qp	31	[258] 5QMAS
	SiOAl O3	3.4	qp	41	[258] 5QMAS
	SiOAl O1	3.5	qp	43.8	[255] 5QMAS
	SiOAl O2	3.6	qp	31.0	[255] 5QMAS
	SiOAl O3	3.4	qp	41.4	[255] 5QMAS
K-A, dehydrated	SiOAl O1	3.7	qp	31.6	[255] 5QMAS
	SiOAl O2	3.7	qp	36.3	[255] 5QMAS
	SiOAl O3	3.5	qp	47.2	[255] 5QMAS
K-A, hydrated	SiOAl O1	3.5	qp	50.9	[255] 5QMAS
	SiOAl O2	3.9	qp	33.9	[255] 5QMAS
	SiOAl O3	3.7	qp	54.8	[255] 5QMAS
Sr-A, hydrated	SiOAl O1	3.7	qp	60.2	[255] 5QMAS
	SiOAl O2	3.9	qp	38.0	[255] 5QMAS
	SiOAl O3	3.6	qp	48.7	[255] 5QMAS
Tl-A, hydrated	SiOAl O1	3.3	qp	60.7	[257]
	SiOAl O2	3.6	qp	53.4	[257]
	SiOAl O3	3.2	qp	75.5	[257]
Na,K-LSX, hydrated	SiOAl O1	3.3	qp	50.6	[257]
	SiOAl O2	3.3	qp	42.1	[257]
	SiOAl O3	3.4	qp	45.2	[257]
	SiOAl O4	3.6	qp	36.8	[257]
Na-LSX, hydrated	SiOSi	5.0	qp	53	[258] 3QMAS
	SiOAl O1	3.2	0.4	50.3	[256]
	SiOAl O1	3.5	qp	49	[258] 5QMAS
	SiOAl O2	3.3	0.3	41.7	[256]
	SiOAl O2	3.3	qp	37	[258] 5QMAS
	SiOAl O3	3.4	0.3	45.0	[256]
	SiOAl O3	3.4	qp	42	[258] 5QMAS
	SiOAl O4	3.6	0.15	36.9	[256]
Na,K-LSX, dehydrated	SiOAl O1	3.2	qp	42.5	[259]
	SiOAl O2	3.3	qp	37.9	[259]
	SiOAl O3	3.3	qp	38.7	[259]
	SiOAl O4	3.3	qp	33.1	[259]
	SiOAl O1	-	-	43.3	[260]
	SiOAl O2	-	-	36.1	[260]
	SiOAl O3	-	-	33.3	[260]
	SiOAl O4	-	-	25.4	[260]
Rb,K-LSX, dehydrated	SiOAl O1	-	-	56.4	[260]
	SiOAl O2	-	-	47.8	[260]
	SiOAl O3	-	-	44.7	[260]
	SiOAl O4	-	-	35.8	[260]

Ga-X		SiOGa	4.0	0.3	28	[261]
		SiOSi	5.0	0.0	50	[261]
		SiOSi	4.6	0.1	44	[224] MAS
Ba, Na-Y, Si/A=2.74, dehydr.		SiOAl	3.4	0.4	40	[224] MAS
		SiOSi	5.1	0.15	52	[224] MAS
Na-Y, dealuminated, dehydr.		SiOSi	5.2	0.2	45	[224] MAS
Na-Y, Si/A=2.74, dehydrated		SiOAl	3.1	0.2	31	[224] MAS
NH_4-Y, Si/A=2.92, dehydr.		SiOAl	3.2	0.2	31	[224] MAS
		SiOSi	5.0	0.1	48	[224] MAS
H-Y, dehydrated	OH δ_{1H}=3.7 ppm		6.0	1.0	21	[262]
	OH δ_{1H}=4.4 ppm		6.2	0.9	24	[262]
		SiO2,3,4-Al	3.7	0.2	27.5	[263]
		SiO1Al	3.5	0.3	33.3	[263]
		SiO2,3,4Si	5.3	0.1	44.0	[263]
		SiO1Si	5.1	0.3	50.0	[263]
Na-ZSM-5, hydrated		SiOSi	5.3	0.12	40.0	[264]
		SiOAl	3.5	0.29	30.0	[264]
H-ZSM-5, dehydrated	OH δ_{1H}=4.2 ppm		7.0	0.75	31	[262]
	OH δ_{1H}=4.2 ppm		6.8	0.5	35	[262]
	OH δ_{1H}=4.2 ppm		5.8	0.6	37	[262]
$Na_6[AlSiO_4]_6 \cdot 8H_2O$ (hydrosodalite)		SiOAl	3.4	qp	39.1	[259]
$Na_6[AlSiO_4]_6$ (dehydr. hydrosodalite)		SiOAl	4.3	qp	36.3	[259]
$Na_8[AlSiO_4]_6(OH)_2 \cdot 2H_2O$ (hydroxosodalite)			3.4	qp	36.0	[259]
$Na_8[AlSiO_4]_6(OH)_2$ (dehydr. hydroxosodalite)			3.5	qp	39.2	[259]
Ga-sodalite		SiOGa	4.0	0.3	29	[261]
		SiOSi	5.1	0.0	52	[261]
Na-Ba-Ga-sodalite		SiOGa	4.0	0.3	29	[261]
		SiOSi	5.1	0.0	52	[261]
$Na_{0.46}Ca_{2.0}Al_{4.5}Si_{13.5}O_{36} \cdot 10.8H_2O$		SiOSi	5.1	0.18	43	[265]
(stilbite)		SiOAl	3.5	0.28	33	[265]
$NaAlSi_2O_6 \cdot H_2O$ (analcime)		SiOSi	5.0	qp	51	[266]
		SiOSi	4.7	qp	51	[258] 5QMAS
		SiOAl	3.1	qp	35	[266]
		SiOAl	3.2	qp	35	[258] 5QMAS
		AlOAl	1.7	qp	26	[266]
		H_2O	6.87	0.67	−15.5	[267]
		H_2O	7.6	0	(−?)18	[268]
$Al_2Si_2O_5(OH)_4$ (kaolinite)		SiOSi O3	4.45	0.43	54.3	[269]
		SiOSi O5	4.65	0.38	51.3	[269]
		SiOSi O4	4.75	0.28	46.5	[269]
		OH	6.9	0.55	41.5	[269]
		SiO2Al	3.4	0.8	6	[269]
$KAl_2[(OH,F)_2/AlSi_3O_{10}]$		SiOSi	4.6	0.5	53.0	[269]
(muscovite)		SiOSi	4.5	qp	53.2	[270]
		SiO2Al	3.5	0.8	66.5	[269]
		SiO2Al	3.5	qp	66.2	[270]
		SiOAl	3.1	0.5	46.2	[269]
		SiOAl	2.89	qp	45.22	[270]
		OH	6.75	0.5	44.5	[269]
		2AlOH	7.4	qp	34	[270]
$NaAlSi_2O_6$ (jadeite)		O1	3.3	0.9	64	[51]
		O2	4.1	0.15	59	[51]
		O3	5.0	0.5	69	[51]

$Mg_3Al_2Si_3O_{12}$ (pyrope)		3.40	0.30	84.0	[51]
$Ca_3Al_2Si_3O_{12}$ (grossular)		4.10	0.40	102.0	[51]
$1.7Al_2O_3{\cdot}SiO_2$ (mullite)	Oc*	2.0	0.4	40.5	[51]
	Oc	3.3	0.1	76	[51]
	Oab and Od	3.3	0.3	58.5	[51]
Yttrium aluminosilicat glass	br O	3.1	-	54	[271]
	nb O			143	[271]
	nb O			210	[271]
Lanthanum aluminosilicat glass	br O	3.1	-	58	[271]
	nb O			178	[271]
$NaAlSi_3O_8$ (glass)	SiOSi	5.1	0.15	49	[272]
	SiOSi	5.2	0.2	40	[242]
	SiOAl	3.2	0.05	33	[272]
	SiOAl	3.8	0.2	25	[242]
Na, $LiAlSiO_4$ (glasses)	SiOSi	≈4.5-5.0	-	≈49-66	[273]
	SiOAl	≈3.0-3.5	-	≈35-42	[273]
	AlOAl	≈1.7-1.9	-	≈18-22	[273]
$14Na_2O{\cdot}4Al_2O_3{\cdot}17B_2O_3{\cdot}65SiO_2$	SiOSi	5.1	qp	40	[274]
(glass)	SiOB	5.2	qp	57	[274]
	BOB	5.6	qp	62	[274]
	SiOAl	3.6	qp	26	[274]
$CaAl_2Si_2O_8$ (glass)	SiOAl	3.5	-	61	[275]
	nb O	2.9	-	113	[275]
Sodium aluminosilicate glass, NAS, Si/Al=0.7	AlOAl	1.85	qp	19	[219]
Calcium aluminosilicate glass, CAS, Si/Al=0.5	AlOAl	2.4	qp	68	[219]
Phosphorous containing materials					
$AlPO_4$-5	AlOP	5.7	0.0	63	[261]
$AlPO_4$-11	AlOP	5.7	0.0	64	[261]
$AlPO_4$-17	AlOP	5.6	0.1	67	[261]
$AlPO_4$-14 as synthesized	AlOP	5.85	0.10	66.8	[276]
	AlOP	5.79	0.13	68.1	[276]
	AlOP	5.82	0.18	75.0	[276]
	AlOP	5.06	0.23	78.8	[276]
	AlOP	4.93	0.41	87.2	[276]
	AlOP	5.27	0.34	97.4	[276]
$AlPO_4$-14 calcined, dehydrated	AlOP	5.86	0.16	59.0	[276]
	AlOP	5.76	0.21	68.8	[276]
h-P_2O_5	br POP	7.46	0.60	122	[277]
	nb PO	3.96	0.00	80	[277]
KH_2PO_4		5.2	0.55	92	[278]
$NH_4H_2PO_4$		5.1	0.55	93	[278]
α/β-$Mg_2P_2O_7$	nb O	5.27	0.40	82.9	[279]
$Na_4P_2O_7$	nb O	3.90	0.6	85.7	[279]
	nb O	3.90	0.6	81.0	[279]
	br O	3.90	0.55	134.3	[279]
$Ba_2P_2O_7$	nb O	4.19	0.26	141.3	[279]
	br O	7.25	0.15	142.9	[279]
	br O	6.82	qp	134.9	[279]
Sodium phosphate glass	br POP	7.7	0.35	119.1	[280]
$51.7Na_2O$ $48.3P_2O_5$	nb PONa	4.8	0.15	84.1	[280]

NaPON glass	PONa	4.4	0.2	8.0	[281]
	PON-1/2/3/4	4.3-4.4	0.1-0.3	12.2-15.8	[281]
Sodium borophosphate glass	nb NaOP	4.2	qp	83	[282]
	br POP	7.9	qp	120	[282]
	nb NaOB	4.7	qp	61	[282]
	br BOP	7.1	qp	93	[282]
$Ca_5(PO_4)_3(OH)$ (hydroxyapatite)	peak 1	4.0	0.0	108	[278]
	peak 2	4.1	0.1	115	[278]
$CaHPO_4 \cdot 2H_2O$	peak 1	4.2	0	98	[278]
	peak 2	4.3	0	96	[278]
Germanium containing materials					
GeO_2 (quartz)	GeO_4	7.3	0.48	70	[283, 284]
	O_{44}	7.05	0.53	49.5	[203]
GeO_2 (rutile)	OGe_3	7.5	0.10	160	[283, 284]
	O_{66}	7.35	0.08	152.2	[203]
GeO_2 (glass)	GeO_4	7.1	0.48	70	[284]
	O_{44}	7.7	qp	42	[203]
$Na_2Ge_2O_5$	nb O	5.95	0.0	38.5	[202]
	O_{44}	6.05	0.6	61	[202]
Na_2GeO_3	GeO_4	5.2	0.5	70	[283]
	O_{44} O1	5.5	0.70	75	[203]
	nb O	2.5	0.5	47	[283]
	nb O1	5.45	0.00	45.5	[203]
$Na_2Ge_4O_9$	O_{44}	5.9	0.54	70.0	[203]
	O_{46} A	5.9	0.48	117.0	[203]
	O_{46} B	5.7	0.48	133.5	[203]
	O_{46} C	6.4	0.65	151.0	[203]
$Na_4Ge_9O_{20}$	O_{44}	6.4	0.65	70.0	[203]
	O_{46}	5.6	0.88	117.0	[203]
	O_{666}	3.75	0.05	133.5	[203]
$Na_2O \cdot 9GeO_2$ (glass)	GeO_4 & GeO_6	7.0	0.5	165	[283]
2 $9GeO_2$ (glass)	GeO_4	6.0	0.5	80	[283]
$14Na_2O \cdot 86GeO_2$ (glass)	O_{44}	7.0	qp	57	[203]
	O_{45}/O_{46}	7.1	qp	97	[203]
	O_{45}/O_{46}	6.3	qp	144	[203]
$27Na_2O \cdot 73GeO_2$ (glass)	nb O	5.9	qp	47	[203]
	O_{44}	6.6	qp	64	[203]
	O_{45}/O_{46}	6.8	qp	105	[203]
$LiTiOGeO_4$	TiOGe	4.8	0.22	148	[247]
$HfGeO_4$ (gel)	HfOGe	5.2	0.65	185	[285]
Others					
H_2O_2 (solution)		-	-	180	[286]
(NQR at 1.5 K)		16.31	0.687	-	[287]
$NaIO_4$		11.19	0.066	250	[288] 19.6 T
KIO_4		10.87	0.032	251	[288] 19.6 T HfO_2 and hafnates
	7 compounds	-	-	237.8-331.9	[285]
	nb apical OTi	≈0	-	749	[247]
$KReO_4$ (perrhenate)		1.28	0.25	137	[289]
NH_4ReO_4 (perrhenate)		1.25	0.16	133	[289]
TiO_2 (rutile)	TiOTi	1.5	0.87	596.5	[290]
	TiOTi	< 1.5	-	590	[217]

(anatase)	TiOTi	< 1.1	-	558	[217]
Ti2O3 (corundum)	TiOTi	< 2.6	-	503	[217]
Li_2O_2	LiOLi	18.0	0.00	227	[291]
Li_2, Ca, Sr, $BaTiO_3$	5 compounds	-	-	372-564	[221]
Li_2, Na_2, Ca, Sr, $BaZrO_3$	5 compounds	-	-	280-376	[221]
Li_2, $SrSnO_3$	3 compounds	-	-	85-423	[221]
$LiNbO_3$		3.4 (maximum)	-	504	[221]
SiO_2/TiO_2 (gel)	SiOSi	5.1	0.0	42	[292]
QTiAc: TEOS, $Ti(OPr^i)_4$, AcacH	SiOTi	2.7	0.0	174	[292]
	SiOTi	3.0	0.0	314	[292]
	nb OTi_4	-	-	375	[292]
	nb OTi_3	-	-	542	[292]
ZrO_2	tetragonal	< 1.4	-	383	[217]
	tetragonal	0.26	0.68	384	[293]
(baddeleyite)	monoclinic	< 0.9	-	325	[217]
	monoclinic	< 1.0	-	402	[217]
ZnO (wurtzite)		< 1.4	-	383	[217]
SnO (litharge)		< 2.3	-	251	[217]
La_2O_3	hexagonal	< 1.4/2.2	-	469/590	[217]
HfO_2 (baddeleyite)		< 1.1	-	267/335	[217]
PbO (litharge)		< 0.9	-	294	[217]
M_xO_y-PDMS-hybrides	SiOTa	3.0	-	243	[294]
	nb OTa_2	-	-	440	[294]
	SiONb	-	-	275	[294]
	nb ONb_2	-	-	545	[294]
	SiOTi	3.0	-	332	[294]
	nb OTi_2	-	-	719	[294]
	SiOZr	3.4	-	219	[294]
	nb OZr_3	-	-	402	[294]
V_2O_5 (crystalline)	O_{1A}	0.9	0.6	1213	[295]
	O_{1B}	4.0	0.7	400	[295]
	O_{1C}	3.3	0.6	0	[295]
$Na_2Al_2B_2O$	O1	3.7	0.77	65.0	[105]
	O2	1.4	0	24.5	[105]
SrB_4O_7	BO	5.50/5.60/5.55	0.25-0.65	79.8/78.2/72.1	[296]
	Tricluster	6.6	0.2	68.0	[296]
Sodium aluminoborate glass	AlOAl	1.7	qp	18.6	[297]
NAB-40-20-40	AlOB	3.7	qp	44.1	[297]
	AlOB	4.1	qp	62.7	[297]
	B nb O	4.0	qp	83	[297]
	BOB	4.8	qp	89	[297]
	BOB	5.0	qp	95	[297]
NAB-30-5-65	AlOB	4.3	qp	61.9	[297]
	B nb O	4.0	qp	83	[297]
	BOB	4.8	qp	87.1	[297]
	BOB	5.4	qp	96	[297]
Borate, borosilicate,	SiOSi	5.4 and 4.9	qp	37 and 51	[298]
boroaluminate glasses	BOB	5.5 and 5.1	qp	92 and 82	[298]
	SiOB	5.6	qp	64	[298]
	Si[B]ONa	2.2	qp	35	[298]
	Si[B]OK	2.1	qp	76	[298]
	AlOB	4.1	qp	59	[298]
	Al[B]ONa	1.7	qp	16	[298]

Titania based hybrids	POTi 4	5.2	0.15	152.5	[299]
	POTi 1-2-3	5.3	0.15	215.0	[299]
$Mg(OH)_2$ (brucite)	MgOH	6.8	0	20	[300]
	MgOH	6.8	0.0	25	[232]
$Mg(OH)_2$	MgOH	6.8	0.0	25	[216]
$Ba(ClO_3)_2{\cdot}H_2O$	H_2O	6.8	1.00	22	[278]
$Ba_2In_2O_5$ (brownmillerite)	site A (O1/O3)	5.0	0.2	189	[301]
	site B (O2)	5.8	0.2	146	[301]
$Ba_2In_2O_4(OH)_2$	site A/ site B	4.5/4.1	0.0/0.7	188/173	[302]
	site C/ site D	4.2/4.8	0.5/0.7	152/97	[302]
$LaSiO_2N$ (La-N-wollastonite)	nb OSi	2.4	-	215	[303]
$La_4Si_2O_7N_2$	ionic	≈0	-	575	[303]
	nb OSi	2.4	-	220	[303]
La_4SiAlO_8N	ionic	≈0	-	570	[303]
	nb OAl	1.8	-	311	[303]
	nb OSi	3.1	-	246	[303]
$La_{10}Si_6O_{24}N_2$	ionic	<1	-	596	[303]
$Na_2(ONNO_2)$		13.5	0.40	265	[304]
$[HONH_3]Cl$		14.7	0.71	90	[304]
LiOH (NQR)		−7.283	0.07	-	[305]
NaOH (NQR at 77 K))		−7.590	0.07	-	[305]
KOH (NQR at 77 K))		−7.140	0.08	-	[305]
β-$Ba(OH)_2$ (NQR at 77 K))		−7.124	0.07	-	[305]
$Sr(OH)_2$ (NQR at 77 K))		−7.267	0.08	-	[305]
$Ca(OH)_2$		6.5	0.00	62	[278]
CaOH		6.5	0.3	71	[228]
$CaCO_3$		6.97	1	204	[306]
ThO_2		very small		576	[307]
UO_2		very small		717	[307]
NpO_2		very small		475	[307]
PuO_2		very small		54	[307]
AmO_2		very small		−754	[307]

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