

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 useful 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 2024:

deuterium-2	1620	calcium-43	964	rubidium-85	7	cesium-133	193
lithium-6	373	scandium-45	113	rubidium-87	98	barium-135	4
lithium-7	1172	titanium-47/49	48	strontium-87	17	barium-137	13
beryllium-9	41	vanadium-50	0	zirconium-91	32	lanthanum-138	1
boron-10	5	vanadium-51	520	niobium-93	93	lanthanum-139	60
boron-11	372	chromium-53	6	molybdenum-95	76	hafnium-177	0
nitrogen-14	532	manganese-55	30	molybdenum-97	0	hafnium-179	0
oxygen-17	1141	cobalt-59	100	technetium-99	20	tantalum-181	2
neon-21	0	nickel-61	4	ruthenium-99	8	rhenium-185/187	10
sodium-23	1169	copper-63/65	121	ruthenium-101	0	osmium-189	0
magnesium-25	139	zinc-67	61	palladium-105	5	iridium-191	0
aluminum-27	5426	gallium-69/71	284	indium-113	9	iridium-193	0
sulphur-33	49	germanium-73	23	indium-115	48	gold-197	13
chlorine-35/37	191	arsenic-75	26	antimony-121	22	mercury-201	4
potassium-39	76	bromine-79	47	antimony-123	5	bismuth-209	14
potassium-40	0	bromine-81	24	iodine-127	46		
potassium-41	0	krypton-83	2	xenon-131	6		

The search string *PY=1950-2024 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 ^2H 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, offered by P. Man on his Internet page www.pascal-man.com. M. E. Smith [2] presented in 2020 a review involving 19 half-integer spin low- γ quadrupolar nuclei in inorganic materials.

Table 8.1. ^{27}Al , quadrupole coupling constant $C_Q = e^2qQ/h$, the asymmetry parameter η , and the isotropic value of the chemical shift δ (referred to 1.0 M $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ [3]) for the ^{27}Al NMR of powder compounds at ambient temperature. The data published from 1983-1992 were compiled by Müller [4]. Chandran *et al.* [5] presented in 2019 a review on ^{27}Al NMR studies of all known transition alumina phases and proposed a new 3D correlative method of NMR parameters, enabling fingerprinting and identification of such phases. It includes the aluminas χ , κ , θ , γ , δ , η , ρ and α -alumina as their final outcome of a calcination above 1350 °C [5]. In 2020, a review on ^{27}Al NMR studies of aluminosilicate glasses was given by Edén [6].

The acronym “qp” appears in the column for η , if the column C_Q 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 compounds without B, C, N, F, Si, P, S						
α -Al(OH) ₃ (bayerite)	AlO ₆	2.9	qp	11	[7]	
	AlO ₆ -(1)	1.4	0.80	13.1	[5, 8]	
	AlO ₆ -(2)	1.9	0.25	9.1	[5, 8]	
γ -Al(OH) ₃ (gibbsite)	AlO ₆ -(1)	2.2	qp	11	[9]	
	AlO ₆ -Al(2)	2.2	0.75	10.5	[8]	
	AlO ₆ -(2)	4.5	0.45	12	[9]	
	AlO ₆ -Al(1)	4.7	1.00	17.2	[8]	
	AlO ₆ -I	4.6	0.4	13.6	[5, 10]	
	AlO ₆ -II	2.2	0.7	11.3	[5, 10]	
α -AlO(OH) (diaspore)	AlO ₆	3.4	0.8	17.0	[5, 11]	
γ -AlO(OH) (boehmite)	AlO ₆	-	-	9 (anisotr.)	[12]	
	AlO ₆	1.8-2.8	0.5-1.0	12.6	[5, 8]	
α -Al ₂ O ₃ (corundum)	AlO ₆	2.40	0.01	18.8	[13]	
α -Al ₂ O ₃	AlO ₆	1.58	qp	10.7	[14]	
	AlO ₆	2.38	0.0	13.5	[5, 15]	
	grain size 12-52 nm	AlO ₆	2.4	0.05	16.0	[5, 16]
	grain size 3.8 nm / 13 nm	AlO ₄	2.4	-	71	[17]
		AlO ₆	2.4	-	14	[17]
γ -Al ₂ O ₃ (non-hydrated)	AlO ₄	8.5	0.8	68	[18]	
	AlO ₆	5.5	0.7	13	[18]	
$\gamma/\delta/\theta$ -Al ₂ O ₃ (calcined)	AlO ₆ ⁽¹⁾	4.9/4.8/4.4	0.0/0.0/0.0	16.9/16.3/15.8	[19]	
	AlO ₆ ⁽²⁾	5.5/4.3/2.9	0.4/0.6/0.3	15.7/14.5/13.2	[19]	
	AlO ₆ ⁽³⁾	4.4/3.5/3.5	0.5/0.5/0.5	11.0/10.8/10.2	[19]	
	AlO ₆ ⁽⁴⁾	6.0/5.9/5.9	0.6/0.6/0.6	8.6/9.8/9.7	[19]	
	AlO ₄ ⁽¹⁾	6.4/6.0/6.2	0.5/0.7/0.7	78.8/80.0/80.3	[19]	
	AlO ₄ ⁽²⁾	6.1/4.6/4.9	0.5/0.6/0.6	73.9/73.2/73.0	[19]	
	AlO ₄ ⁽³⁾	6.6/6.6/6.6	0.6/0.4/0.4	67.5/68.3/66.7	[19]	
γ -Al ₂ O ₃ (hydrated)	AlO ₄	5.1	-	71.5	[20]	
	AlO ₅	5.1	-	44.0	[20]	
	AlO ₆	3.55	-	10.0	[20]	
	grain size 3.8 nm / 13 nm	AlO ₄	0.06	-	63	[17]
		AlO ₅	0.06	-	43	[17]
		AlO ₆	0.06	-	7	[17]
γ -Al ₂ O ₃ (dehydrated, needles)	AlO ₄	15.5	0.1	82	[21]	
	AlO ₄	13.2	0.5	72	[21]	
	AlO ₆	11.8	0.5	18	[21]	
η - Al ₂ O ₃ size 3.8 nm / 13 nm	AlO ₆	0.08	-	-6	[17]	
ρ -Al ₂ O ₃	AlO ₄ , AlO ₅ , AlO ₆	insufficiently resolved			[22]	

κ -Al ₂ O ₃	AlO ₄	7.6	0.3	81.5	[23]
	AlO ₆ -(1)	5.0	-	ca. 13	[23]
	AlO ₆ -(4)	8.5	-	18	[23]
χ -Al ₂ O ₃ (part. dehydr. gibbsite)	AlO ₄	5.0	0.3	71.5	[24]
	AlO ₅	2.7	0.3	38.5	[24]
	AlO ₆	4.5	0.3	11.5	[24]
θ -Al ₂ O ₃	AlO ₄	6.4	0.65	80	[15]
	AlO ₆	3.5	0	10.5	[15]
η -, γ -, δ -, θ -Al ₂ O ₃	AlO ₄	4.7-5.5	0.4-0.8	74-80	[25]
	AlO ₆	3.0-4.0	0.4	11-15	[25]
CaO·6Al ₂ O ₃	AlO ₄	2.0	0 _{assumed}	65	[26]
	AlO ₅	6.7	0 _{assumed}	27.5	[27]
	AlO ₆ -(1)	1.5	0 _{assumed}	9	[26]
	AlO ₆ -(2)	<1	0 _{assumed}	16	[26]
CaO·2Al ₂ O ₃	AlO ₄ -(1)	6.7	0.8	78	[26]
	AlO ₄ -(2)	13	0.1	ca. 60	[26]
CaO·Al ₂ O ₃	AlO ₄ -(1)	2.7	0.85	80	[26]
	AlO ₄ -(2)	2.7	0.85	83	[26]
4CaO·3Al ₂ O ₃	AlO ₄	2.4	0.95	80	[26]
12CaO·7Al ₂ O ₃	AlO ₄ -(1)	3.7	0.9	79	[26]
	AlO ₄ -(2)	11	0.2	85	[28]
3CaO·Al ₂ O ₃	AlO ₄	9.7	0.3	85	[28]
	AlO ₄ -(1)	8.69	0.32	79.5	[29]
	AlO ₄ -(2)	9.3	0.54	78.25	[29]
4CaO·3Al ₂ O ₃ ·3H ₂ O	AlO ₄ -(1)	1.8	0.5	78	[26]
	AlO ₄ -(2)	5.4	0.45	79	[26]
CaAl ₄ O ₇	AlO ₄ -(1)	6.25	0.88	75.5	[30]
		6.4	0.90	68.1	[31]
	AlO ₄ -(2)	9.55	0.82	69.5	[30]
		9.5	0.82	59.1	[31]
CaAl ₁₂ O ₁₉	site 1/2	3.2/4.2	0.0/0.0	65.7/20.0	[31]
	site 3/4/5	4.5/-/-	0.9/-/-	18.0/13.6/6.7	[31]
	site 1/2	0.15/21.4	-/0.00	16.25/55.8	[32]
	site 3/4/5	3.1/1.6/4.8	0.00/-/0.7	68.1/9.92/22.3	[32]
SrAl ₁₂ O ₁₉	site 1/2	0.25/20.75	-/0.00	16.72/57.8	[32]
	site 3/4/5	3.45/1.35/4.9	0.00/-/0.65	67.5/9.45/22.1	[32]
	AlO ₄ /AlO ₄ -d	3.455/20.71	0.5/0.00	67.90/56.91	[33]
	AlO ₅	2.590	qp	19.50	[33]
	AlO ₆ -1/2	17.50/10.06	qp/qp	17.50/10.06	[33]
	AlO ₆ -3	4.990	0.65	21.73	[33]
LaSrAl ₃ O ₇	site 1	3.0	0.5	75.4	[34]
	site 2	6.8	0.5	83.3	[34]
LaSrAl _{1.5} Ga _{1.5} O ₇	site 1	4.2	0.5	78.7	[34]
	site 2	7.0	0.5	83.8	[34]
CaAl ₂ O ₄	AlO ₄ -(1-5)	2.4-4.2	0.2-0.95	81.2-86.2	[30]
Ca ₁₂ Al ₁₄ O ₃₃	AlO ₄ -(1)/(2)	9.7/3.8	0.4/0.7	85.9/80.2	[30]
Ca ₃ Al ₂ O ₆	AlO ₄ -(1)/(2)	8.69/9.3	0.32/0.54	79.5/78.3	[30]
CaAl ₂ H ₂₀ O ₁₄	AlO ₆	2.4	qp	10.2	[30]
Ca ₃ Al ₂ H ₁₂ O ₁₂	AlO ₆	0.705	0.09	12.36	[30]
Ca ₄ Al ₂ H ₂₆ O ₂₀	AlO ₆	1.8	qp	10.2	[30]
KAlO ₂	AlO ₄	1.1	0.7	76	[28]
KAlO ₂ ·0.5H ₂ O	AlO ₄	5.6	0.0	77	[28]
KAlO ₂ ·H ₂ O	AlO ₄	6.5	0.6	83	[28]

KAlO ₂ ·1.5H ₂ O	AlO ₄	5.0	0.25	81	[28]
5BaO·Al ₂ O ₃	AlO ₄	2.3	0.8	80	[28]
BaO·Al ₂ O ₃	AlO ₄	2.4	0.4	78	[28]
α-BaO·Al ₂ O ₃ ·2H ₂ O	AlO ₄ -(1)/(2)	3.4/5.1	0.5/0.9	81/80	[28]
α-LiAlO ₂	AlO ₆	2.8	0.05	16	[35]
β-LiAlO ₂	AlO ₄	1.8	0.55	82	[35]
	AlO ₄	1.86	0.56	83.0	[36]
γ-LiAlO ₂	AlO ₄	3.2	0.7	81	[35]
single crystal	AlO ₄	3.330	0.656	81.8	[37]
β-NaAlO ₂	AlO ₄	1.4	0.5	80	[28]
NaAl ₉ O ₁₄	AlO ₄	3.4	qp	55.9	[38]
	AlO ₆	2.8	qp	9	[38]
AlCl ₃ ·3Al(OH) ₃ ·6H ₂ O	AlO ₆	6.9	0.4	7	[4]
AlCl ₃ ·4Al(OH) ₃ ·7H ₂ O	AlO ₆	5.7	0.7	3	[4]
AlCl ₃ ·OPCl ₃	AlCl ₃ O	6.0	0.15	88	[39]
Al ₂ Ge ₂ O ₇	AlO ₅	8.8	0.4	36	[40]
AlLaGe ₂ O ₇	AlO ₅	7.2	0.37	36	[40]
Al ₂ (MoO ₄) ₃	AlO ₆ -(1)/(2)	1.12/0.88	0.65/0.95	-12.4/-13.4	[41]
	AlO ₆ -(3)/(4)	1.21/0.78	1.0/0.8	-10.3/-11.1	[41]
MgAl ₂ O ₄ (spinel)	AlO ₄	3.2	0.50	76.5	[42]
	AlO ₆ -1	3.73	0.26	14.5	[42]
	AlO ₆ -2	4.46	0.4	-1.0	[42]
Cd ₈ (AlO ₂) ₁₂ S ₂ (sodalite)	AlO ₄	2.00	< 0.1	80.4	[43]
Ca ₈ (AlO ₂) ₁₂ S ₂ (sodalite)	AlO ₄	3.55	< 0.1	79.1	[43]
Cd ₈ (AlO ₂) ₁₂ Se ₂ (sodalite)	AlO ₄	3.95	< 0.1	78.7	[43]
Cd ₈ (AlO ₂) ₁₂ (SO ₄) ₂ (sodalite)	AlO ₄	3.24	< 0.1	79.1	[43]
Sr ₈ (AlO ₂) ₁₂ S ₂ (sodalite)	AlO ₄	4.65	< 0.1	76.9	[43]
Sr ₈ (AlO ₂) ₁₂ Se ₂ (sodalite)	AlO ₄	5.10	< 0.1	76.6	[43]
Sr ₈ (AlO ₂) ₁₂ (CrO ₄) ₂ (sodalite)	AlO ₄	6.75	< 0.1	75.5	[43]
SrAl ₁₂ O ₁₉	AlO ₄	3.45	0.1	68.0	[44]
	AlO ₅	2.1	0.7	18.0	[44]
	AlO ₆ -(1)	0.6	1	17.1	[44]
	AlO ₆ -(2)	1.3	1	9.6	[44]
	AlO ₆ -(3)	4.9	0.63	21.7	[44]
Sr ₄ Al ₁₄ O ₂₅	Al1/Al2/Al3	4.4/5.2/4.2	0.8/0.8/0.2	78/82/77	[45]
	Al4/Al5/Al5	2.4/6.8/9.2	0.1/0.2/0.0	12/12/11	[45]
YAlO ₃	AlO ₆	1.61	qp	10.7	[14]
Y ₄ Al ₂ O ₉	AlO ₄ -1	10.81	0.48	78.2	[14]
	AlO ₄ -2	10.36	0.77	76.2	[14]
Y ₃ Al ₅ O ₁₂	AlO ₆	1.13	qp	2.1	[14]
	AlO ₄	6.21	0.05	77.5	[14]
	AlO ₆	1.13	qp	2.1	[14]
Y ₃ Al ₅ O ₁₂ (YAG II 800)	AlO ₆ /AlO ₅	-	-	1.2/23.6	[46]
	AlO ₄	6.0	0.08	76.6	[46]
Y ₃ Al ₅ O ₁₂ (YAG)	AlO ₆	0.6	-	5.38	[47]
	AlO ₄	6.1	-	82	[47]
AlVO ₄	Al1	1.64	0.30	-8.9	[48]
	Al2	6.73	0.42	27.2	[48]
	Al3	5.88	0.58	-1.1	[48]
ZrO ₂ -Al ₂ O ₃ (co-hydrolysis, annealed at 1000 °C)	AlO ₄ / AlO ₅	10.0/5.0	-	78/37	[49]
	AlO ₆	7.0	-	16	[49]

MgO-Al ₂ O ₃ (annealed 600 °C)	AlO ₄ / AlO ₅	10.5/10.0	-	82/41	[49]
	AlO ₆	7.0/2.0	-	17/15	[49]
CsAlH ₄ orthorhombic	MAS/static	1.42/1.42	0.60/0.62	121.4/122	[50]
CsAlH ₄ tetragonal	MAS/static	1.42/1.43	<0.05/<0.03	116.8/116	[50]
KAlH ₄	MAS/static	1.29/1.30	0.64/0.64	107.6/108	[51, 52]
NaAlH ₄	MAS/static	3.11/3.11	<0.05/0.01	97.2/99	[51, 52]
NaAlH ₄		3.15	0.04	97.5	[53]
Na ₃ AlH ₆ doped/non-doped		0.52/0.70	0.5/0.2	-42.7/-42.5	[53]
Na ₂ LiAlH ₆		<0.1	-	-46	[53]
ZrNiAl	Al-Ni	3.3	0.42	393	[54]

Zeolites and zeolite-like materials

Zeolite Na-A (hydrated)	AlO ₄	1.1	0.75	59.2	[55]
Zeolite H, Na-A (dehydrated)	AlO ₃	12	-	-	[56]
Zeolite Na-Y (hydrated)	AlO ₄	2.0	0.5	62.8	[55]
Zeolite Na-Y (dehydrated)	AlO ₄	5.5	0.3	ca. 60	[57]
Zeolite H-Y (dehydrated)	AlO ₃	13.1	0.75	105±20	[57]
	AlO ₃	15.3	0.4	60	[58]
Zeolite Al, Na-Y (dehydrated)	AlO ₄ /Al ^{x+}	14.5	0.3	70	[18]
	AlO ₄ /Na ⁺	5.5	0.8	60	[18]
	Al ^{x+} cat.	6.0	0.7	35	[18]
Zeolite H, Na-Y (hydrated)	AlO ₄ /H ⁺	16.0/14.0	0.3	70	[18]
	AlO ₄ /Na ⁺	5.5	0.8	60	[18]
Dealumin. H, Na-Y (hydr.)	AlO ₄ /H ⁺	15.0	0.3	70	[18]
	AlO ₄ /Na ⁺	8.0	0.8	65	[18]
	Al ^{x+} cat.	7.5	0.7	35	[18]
	AlO ₆ cluster	5.0	0.7	10	[18]
Zeolite USY (hydrated)	AlO ₄ /AlO ₅ /AlO ₆	2.8/4.1/2.9	-	60.0/34.5/4.0	[20]
	AlO ₄ (4 sampl.)	1.9-7.5	qp	60.5-69.7	[59]
	AlO ₅ (4 sampl.)	3.9-4.6	qp	34.0-39.8	[59]
	AlO ₆ (4 sampl.)	1.9-3.2	qp	0.1-7.5	[59]
Zeolite Y, dealuminated	AlO ₅ -1/2	5.0/5.6	-	29/35	[60]
	AlO ₄ -1/2/3	15.0/4.2/11.2	-	57/58/60	[60]
Zeolite Ti-USY	AlO ₄	2.0/1.5	qp/qp	64.4/61.1	[61]
	AlO ₅	3.2	qp	33.9	[61]
	AlO ₆	2.0/1.6	qp/qp	6.0/0.01	[61]
Zeolite H-MOR (dehydrated)	AlO ₃	15.0	0.35	-	[62]
	AlO ₄	6.8	0.7	-	[62]
Zeolite MOR (dehydrated)	AlO ₄	14	-	58	[21]
	AlO ₄	19	-	57	[21]
Zeolite NH ₃ (H)-MOR	AlO ₄ (NH ₄)/(H)	1.9/5.6	qp/ qp	45/35	[63]
Zeolite BEA (Si/Al=9-215)	Td1	2.3-2.5	qp	57.5-59.0	[64]
	Td2	1.7-1.9	qp	53.5-54.0	[64]
Zeolite H-BEA (Si/Al=9-215)	Td1	1.0-2.0	qp	58.5-60.0	[64]
	Td2	1.1-1.7	qp	55.0-60.0	[64]
Zeolite H-BEA (dehydrated)	AlO ₃	16	0.1	-	[56]
Zeolite BEA (3 samples)	AlO ₄ (2b)	2.3-2.4	qp	58.0-58.4	[65]
	AlO ₄ (2a)	1.5-1.8	qp	53.9-54.2	[65]
	AlO ₆	-	-	≈0	[65]
Zeolite H-BEA	Al'+CD3CN	14	0.7	70	[66]
	Al'+H ₂ O	13	0.9	70	[66]
	SiOHAl	3.5	0.85	60	[66]
	Penta-co. Al	3.5	0.5	40	[66]

Zeolite Na-ZSM-5 (dehydrated)	AlO ₄	4.7	0.5	≈60	[57]
Zeolite H-ZSM-5 (dehydrated)	AlO ₃	16.0	0.1	82±20	[57]
	AlO ₃	15.5	0.5	-	[62]
	AlO ₄	7.3	0.7	-	[62]
Zeolite H-ZSM-5 (dehydrated)	AlO ₄ -1	17.5	0.1	-	[67]
	AlO ₄ -2	11.0	0.6	-	[67]
Zeolite H-ZSM-5 (dehydrated)	AlO ₄	16.1/11.1	0.16/0.66	53.7/57.7	[68]
Zeolite ZSM-5 Si/Al=14-250, 7 samples	AlO ₄ , Peak I	1.6-1.7	qp	54.4-55.7	[69]
	AlO ₄ , Peak II	1.5-1.6	qp	52.2-52.3	[69]
Zeolite TPA-ZSM-5	AlO ₄ (1)/(2)	1.4/1.8	qp/ qp	52.2/54.9	[70]
Zeolite H-ZSM-5	AlO ₄ (1)/(2)	1.2/1.6	qp/ qp	55.5/56.5	[70]
Zeolite NH ₃ (H)-ZSM-5	AlO ₄ (1)/(2)	1.2/1.6	qp/ qp	53.8/56.4	[70]
Zeolite ZSM-23	AlO ₄ (1)-(5)	1.6-2.6	qp	54.4-58.0	[71]
Zeolite TNU-9	AlO ₄	2.1-2.3	qp	53.5-57.2	[72]
Zeolite Li-CHA (hydrated)	AlO ₄	2.4	qp	60.0	[73]
Zeolite Li-CHA (dehydrated)-I	AlO ₄	5.3	qp	62	[73]
Zeolite Li-CHA (dehydrated)-II	AlO ₄	7.3	qp	57	[73]
Zeolite Na-CHA (hydrated)	AlO ₄	1.8	qp	59.5	[73]
Zeolite Na-CHA (dehydrated)	AlO ₄	4.2	qp	61	[73]
Zeolite K-CHA (hydrated)	AlO ₄	1.8	qp	59.5	[73]
Zeolite K-CHA (dehydrated)	AlO ₄	2.9	qp	60	[73]
Zeolite ITQ-33	T4	1.11/1.12	qp	52.38/53.46	[74]
	T3	2.20/2.21/2.19	qp	60.75/62.07/63.22	[74]
AlPO ₄ -5 (hydrated)	AlO ₄	2.3	0.95	40.4	[75]
AlPO ₄ -8 (dehydrated)	AlO ₄ -(1)/(2)	3.9/3.6	0.5 _{ass.} / 0.5 _{ass.}	40.1/40.6	[76]
	AlO ₄ -(3)/(4)	3.6/3.0	0.5 _{ass.} / 0.5 _{ass.}	47.0/42.9	[76]
	AlO ₄ -(5)	3.4	0.5 _{assumed}	42.6	[76]
AlPO ₄ -14 (hydrated)	AlO ₅ -(Al1 [77])	5.66	0.89	27.2	[78]
	AlO ₅ -(3)(Al1 [77])	5.58	0.97	27.1	[79]
	AlO ₅ -Al1	5.6	1.0	27	[80]
	AlO ₄ -(Al2 [77])	4.15	0.82	44.0	[78]
	AlO ₄ -(2)(Al2 [77])	4.08	0.82	43.5	[79]
	AlO ₄ -Al2	4.1	0.8	44	[80]
	AlO ₄ -(Al3 [77])	1.75	0.70	43.2	[78]
	AlO ₄ -(1)(Al3 [77])	1.74	0.63	42.9	[79]
	AlO ₄ -Al3	1.7	0.6	43	[80]
	AlO ₆ -(Al4 [77])	2.60	0.68	-0.9	[78]
	AlO ₆ -(5)(Al4 [77])	2.57	0.7	-1.3	[79]
	AlO ₄ -Al4	2.6	0.7	-1	[80]
AlPO ₄ -14 (dehydrated)	AlO ₄ -Al1	4.0	0.8	43	[80]
	AlO ₄ -Al2	3.4	0.2	43	[80]
	AlO ₄ -Al3	2.5	0.6	38	[80]
	AlO ₄ -Al4	4.9	0.3	45	[80]
AlPO ₄ -14A (dehydrated)	AlO ₄ -Al1	4.5	-	63.4	[81]
	AlO ₄ -Al2	4.1	-	43.1	[81]
	AlO ₄ -Al3	4.7	-	45.5	[81]
	AlO ₄ -Al4	2.6	-	-14.9	[81]
AlPO ₄ -15	Al1	3.1	0.8	2.5	[82]
	Al2	3.1	0.8	-5.0	[82]
AlPO-CJ19 (NH ₄) ₂ Al ₄ (PO ₄) ₄ (HPO ₄)·H ₂ O	Al(1)	3.8	-	47.6	[83]
	Al(2)	4.2	0.1	17.0	[83]
	Al(3)	1.4	-	-13.4	[83]
	Al(4)	2.6	-	48.1	[83]

AlPO ₄ -21 (hydrated)	AlO ₄	8.3	0.15	47.3	[84]
	AlO ₅ -(1)/(2)	5.9/7.4	0.68/0.52	14.6/15.7	[84]
AlPO ₄ -25 (hydrated)	AlO ₄ -(1)/(2)	1.9/0.8	0.67 _{ass.} /0.67 _{ass.}	40.8/39.5	[84]
AlPO ₄ -25 (dehydrated)	AlO ₄ -(1)	2.3/1.1	0.67 _{ass.} /0.67 _{ass.}	39.2/37.5	[84]
AlPO ₄ -34 (six samples)	Al1 _{octa}	1.3-2.2	qp	-5.1--4.0	[85]
	Al2 _{tetra}	2.0-2.9	qp	42.7-46.7	[85]
	Al3 _{zetra}	2.5-4.4	qp	46.0-48.0	[85]
AlPO ₄ -53 (hydr. and dehydr.)	sites Al1-Al6	2.0-9.2	0-0.9	17-45	[86]
AlPO ₄ -ZON	site Al1	3.8	qp	50.6	[87]
	site Al2	3.6	qp	43.0	[87]
	site Al3	4.9	qp	27.2	[87]
	site Al4	6.3	qp	24	[87]
AlPO ₄ -SOD as-synthesized dehydrated at 200 °C	Al1/2/3	2.3/2.4/2.7	0.79/0.79/0.82	38/41/-8.5	[88]
	Al1/2/3	2.6/2.8/2.6	0.99/0.42/0.92	39/37/36	[88]
	Al4/5	2.7/2.4	0.35/0.98	12/-12	[88]
AlPO ₄ -STA-1	Al1/2	3.67/4.13	0.39/0.59	45.3/42.2	[89]
	Al3/4	3.84/4.81	0.93/0.90	49.2/43.3	[89]
AlPO ₄ -STA-2	Al1/Al2	2.0/3.5	0.7/0.9	36.0/42.0	[90]
	AlO ₄ 3 sites	2.4/3.6/2.1	qp/qp/qp	39/45/49	[91]
	AlO ₅	3.1	qp	17	[91]
K ₇ Na-JBW (Na ₂ Rb-[AlGeO ₄] ₃ ·H ₂ O)	AlO ₄	1.8	0.69	61.7	[92]
Na ₈ Cl ₂ [Al ₆ Si ₆ O ₂₄] (NaCl-sodalite)		0.7	qp	64.7	[93]
Na ₈ Cl ₂ [Al ₆ Si ₆ O ₂₄] (blue sodalite)	AlO ₄	1.45	0.1	40	[94]
Na _{8.0} Cl _{1.8} [AlSiO ₄] ₆ · 0.4 H ₂ O	AlO ₄	0.94	0.32	62.9	[95]
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄] (NaBr-sodalite)		0.8	qp	63.2	[93]
Na ₈ I ₂ [Al ₆ Si ₆ O ₂₄] (NaI-sodalite)		0.6	qp	61.2	[93]
Na ₈ [Al ₆ Si ₆ O ₂₄]·(H ₃ O ₂) ₂ (basic sodalite)		0.8	qp	64.5	[96]
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄] · (basic sodalite)		0.8	qp	63.4	[96]
Na _{7.7} Br _{1.8} [AlSiO ₄] ₆ · 0.4 H ₂ O	AlO ₄	0.81	0.29	61.8	[95]
Na ₆ [Al ₆ Si ₆ O ₂₄]·(4H ₂ O) ₂ (hydro sodalite)		2.2	qp	65.6	[96]
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄] (dry sodalite)		0.8	qp	63.4	[96]
Li _{7.6} Na _{0.4} Cl _{1.9} [AlSiO ₄] ₆ · 0.7 H ₂ O	AlO ₄	0.98	0.59	71.9	[95]
Li _{7.3} Na _{0.3} Br _{1.8} [AlSiO ₄] ₆ · 1.1 H ₂ O	AlO ₄	0.71	0.61	70.9	[95]
Na _{7.8} I _{1.7} [AlSiO ₄] ₆ · 0.6 H ₂ O	AlO ₄	0.57	0.34	60.4	[95]
Ca ₈ (OH) ₈ Al ₈ Si ₄ O ₂₄ (sodalite)	AlO ₄	5.3	0.24	-	[97]
Na ₆ [AlSiO ₄] ₆ (sodalite)		2.7	O _{assumed}	54	[98]
Na ₆ Zn ₂ [AlSiO ₄] ₆ (SO ₄) ₂ (sodalite)		2.5	O _{assumed}	58	[98]
Other (non-zeolite) aluminosilicates					
H, Al-MCM-41 (as synthesized)	AlO ₄	2.3	O _{assumed}	52.6	[99]
Al ₂ O ₃ -B ₂ O ₃ -SiO ₂ -Na ₂ O glasses		3.7-4.2	qp	59-63	[100]
0.5Al ₂ O ₃ -xSiO ₂ glasses with 1 ≤ x ≤ 6	AlO ₄	5.3-6.5	qp	59-68	[88]
	AlO ₅	4.6-5.3	qp	32-37	[88]
	AlO ₆	3.9-4.6	qp	3-6	[88]
Na ₂ O-CaO-Al ₂ O ₃ -SiO ₂ glass ANCS	AlO ₄	6.8	-	60.5	[101]
	AlO ₅	7.4	-	34.7	[101]
Al ₂ Si ₂ O ₅ (OH) ₄ (kaolinite)	AlO ₆	3.6	qp	7	[9]
	AlO ₆ (1)/(2)	3.4/3.0	0.8/0.9	7.5/8.0	[102]
Al ₂ SiO ₅ (sillimanite)	AlO ₄	6.77	0.53	64.5	[55]
	AlO ₄	6.74	0.51	63.9	[103]
	AlO ₆	8.93	0.46	4.0	[55]
	AlO ₆	8.83	0.49	4.7	[103]
Al ₂ SiO ₅ (andalusite)	AlO ₅ /AlO ₆	5.6/15.3	0.76/0.13	35.2/11.9	[104]

Al ₂ SiO ₅ (kyanite)	AlO ₆ -(1)/(2)	10.1/3.8	0.27/0.85	13.0/4.0	[104]
	AlO ₆ -(3)/(4)	6.4/9.2	0.70/0.38	5.7/5.9	[104]
Al ₄ Si ₈ O ₂₀ (OH) ₄ (pyrophyllite) dehydroxylate (550 °C)	AlO ₆			4.3	[105]
	AlO ₅	10.5	0.6	29	[105]
K _{1.5} Al ₄ (Si _{6.5} Al _{1.5})O ₂₀ (OH) ₄ (illite)	AlO ₄	2.9	-	72.4	[106]
	AlO ₆	3.7	-	6.0	[106]
3Al ₂ O ₃ ·SiO ₂ (mullite)	AlO ₆	7.3	0	6.3	[107]
	AlO ₄ (T)/(T')	7.3/6	0/0.5	68/53	[107]
	AlO ₄ (T*)	4	0.5	45	[107]
2Al ₂ O ₃ ·SiO ₂ (2:1 mullite)	AlO ₆ site 1	4.5	qp	7.5	[108]
	site 2	3.2	qp	49	[108]
	AlO ₄ site 3	4.6	qp	69.4	[108]
3Al ₂ O ₃ ·2SiO ₂ (mullite precursor obtained by sol-gel synthesis)	site 1a/1b	4.3/3.4	qp/qp	7/15	[109]
	site 2	4.3	qp	37	[109]
	site 3	4.1	qp	71	[109]
Mg ₃ Al ₂ Si ₃ O ₁₂ (pyrope)		1.0	0.5	2.9	[110]
Ca ₃ Al ₂ Si ₃ O ₁₂ (grossular)		3.7	0.2	-3.35	[110]
Ca ₂ Al ₃ Si ₃ O ₁₂ -(OH) (zoisite)	AlO ₆ 1/2	7.9/18.4	0.51/0.16	10.7/8.0	[111]
	AlO ₆ 1/2	8.0/18.19	0.53/0.13	10.7/7	[112]
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	[113]
	AlO ₄ d/e	5.4/11.8	0.5/0.45	66.5/79.7	[113]
Sr ₃ Al ₁₀ SiO ₂₀	Al(1)/ Al(2)	3.73/8.13	0/0.3	7.2/12.0	[114]
	T ₂ (4Al)	2.61	0	82.0	[114]
	T ₁ +T ₂ (nAl, mSi)	6.86	0.3	78.0	[114]
(Mg,Fe,Al) ₆ (Si,Al) ₄ O ₁₁ (OH) ₈ (pennine, penninite)	AlO ₄	2.8	-	72	[55]
	AlO ₆	1.4	-	10	[55]
KAlSi ₂ O ₆ (leucite)	T1/T2/T3	2.07/2.58/2.34	qp	61.0/63.9/69.2	[115]
CaAl ₂ Si ₂ O ₈ (anorthite)	6 sites	2.7-8.2	0.45-0.70	61-66	[115]
Na ₁₆ Ca ₁₆ (AlO ₂) ₄₈ (SiO ₂) ₇₂ (mesolite)	Al(1)	3.0	0	64.4	[116]
	Al(2)/ Al(3)	1.9/2.0	0/0	62.6/65.1	[116]
KAl ₂ [(OH,F) ₂ /AlSi ₃ O ₁₀] (muscovite)	AlO ₄	2.1	-	72	[55]
	AlO ₆	2.2	-	5	[55]
CaAl ₂ [(OH) ₂ /Al ₂ Si ₂ O ₁₀] (margarite)	AlO ₄	4.2	-	76	[55]
	AlO ₆	6.3	-	11	[55]
CaMg ₃ Al ₂ Si ₂ O ₁₀ (OH) ₂ (xantophyllite)	AlO ₄	2.8	-	76	[55]
	AlO ₆	2.0	-	11	[55]
Na ₈ Al ₂ Be ₂ Si ₈ O ₂₄ Cl ₂ (tugtupite)	AlO ₄	1.36	0.08	63.4	[117]
NaAlSi ₃ O ₈ (low albite)	AlO ₄	3.29	0.62	62.7	[118]
Na ₂ Al ₂ Si ₃ O ₁₀ ·2H ₂ O (natrolite)	AlO ₄	1.67	0.50	64	[55]
Na ₂ Al ₂ Si ₃ O ₁₀ ·2H ₂ O (tetranatrolite)	AlO ₄ T1/T2	2.2/2.4	qp/qp	63.1/64.2	[119]
KAlSi ₃ O ₈ (microcline)	AlO ₄	3.22	0.21	58.5	[118]
Na,K AlSi ₃ O ₈ (feldspar)	8 samples	3.15-4.0	0.25-0.52	59.2-61.0	[120]
(Mg, Fe)Al ₃ SiBO ₉ (grandidierite)	AlO ₅	8.7	0.95	41.0	[121]
	AlO ₆ -(1)/(2)	3.5/8.6	0.5/0.95	9.0/11.0	[121]
NaCa ₂ Mg ₄ Al(Si ₆ Al ₂)O ₂₂ (OH) ₂ (pargasite)	AlO ₄ (Q ³)	4.0	qp	77	[122]
	AlO ₄ (Q ²)	3.0	qp	76	[122]
NaCa ₂ Mg ₅ Al(Si ₇ Al)O ₂₂ F ₂ (fluor edenite)	AlO ₄ (Q ³)	5.9	qp	77	[122]
Other (non-zeolite) phosphorous containing materials					
AlPO ₄ (quartz)	AlO ₄	4.2	0.35	44.8	[75]
AlPO ₄ (tridimite)	AlO ₄	0.75	0.95	39.8	[75]
AlPO ₄ (cristobalite)	AlO ₄	1.2	0.75	42.5	[75]

$\text{Al}_2\text{PO}_4(\text{OH})_3$ (augelite)	$\text{AlO}_5/\text{AlO}_6$	5.5/4.7	0.78/0.2	30/-3	[123]
$\text{Al}_2\text{PO}_4(\text{OH})_3 \cdot \text{H}_2\text{O}$ (senegalite)	AlO_5	2.87	0 _{assumed}	30	[123]
	AlO_6	4.09	0 _{assumed}	1.7	[123]
KAlP_2O_7	AlO_6	1.2	0.25	-16	[124]
$\text{Zn}_3\text{Al}_6(\text{PO}_4)_{12}$	site 1/ site 2	1.6/1.23	0.4/0.6	49.74/47.6	[125]
Layered aluminophosphates	6 sites	1,3-5.8	0.1-1.0	-17.6-48.1	[126]
$x\text{Al}_2\text{O}_3 \cdot (30-x)\text{P}_2\text{O}_5 \cdot 70\text{SiO}_2$ x=2.5-27.5% (glass)	AlO_4	4.0-6.3	qp	40.1-61.5	[127]
	AlO_5	4.0-6.0	qp	9.4-35.0	[127]
	AlO_6	4.0-5.0	qp	-20.4-5.0	[127]
$\text{AlPW}_{12}\text{O}_{40}$ dehydrated at 473 K	AlO_6	2.4/6.0	1/0.8	2/4	[128]
	AlO_5	7.0/8.7	0.2/0.2	24/44	[128]
	AlO_4	8.5	0.8	65	[128]
60 NaPO_3 40 AlF_3 glass	$\text{Al}^{(6)}/\text{Al}^{(5)}/\text{Al}^{(4)}$	5.1/6.0/3.3	-	-4.5/19/44	[129]

Boron containing materials

AlB_2		0.533	-	880	[130]
$2\text{SrO} \cdot \text{Al}_2\text{O}_3 \cdot \text{B}_2\text{O}_3$	AlO_4	4.3	0.65	83.5	[131]
$2\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot \text{B}_2\text{O}_3$	AlO_4	6.25	0.45	79.5	[131]
$2\text{Li}_2\text{O} \cdot \text{Al}_2\text{O}_3 \cdot \text{B}_2\text{O}_3$	AlO_4	6.0	0.45	76	[131]
$3\text{Li}_2\text{O} \cdot \text{Al}_2\text{O}_3 \cdot 2\text{B}_2\text{O}_3$	AlO_4	6.7	0.83	70	[131]
$9\text{Al}_2\text{O}_3 \cdot 2\text{B}_2\text{O}_3$	AlO_4	6.8	0.1	53	[131]
	AlO_5	4.8	0.3	31	[131]
	AlO_6	6.2	0.4	10.5	[131]
SnAlBO_4 (mullite structure)	$\text{AlO}_{4 \text{ or } 5}$	11.5	0.5	20.6	[132]
	AlO_6	8.8	0.2	22.1	[132]
	$\text{AlO}_{4 \text{ or } 5}$	5.1	0.2	51.5	[132]
$\text{Al}_{6-x}\text{B}_x\text{O}_9$ (mullite structure) 8 samples with $1 \leq x \leq 4$	$\text{AlO}_{4 \text{ or } 5}$	3.9-9.0	-	33.0-67.8	[133]
	AlO_6	4.0-10.5	-	5.1-21.9	[133]
$\text{Na}_2\text{Al}_2\text{B}_2\text{O}$	AlO_4	1.65	0.05	70.3	[134]
$\text{Li}_6\text{Al}_2(\text{BO}_3)_4$		6.4	0.88	69.3	[135]

Flour containing materials

AlF_6^{3-} octahedrons, fluoroaluminates		0.065-1.58	0-0.95	-7-1	[136, 137]
AlF_3		0.213	0.0	-	[138]
$\alpha\text{-AlF}_3$	AlF_6	2.8	0	-13.2	[139]
$\beta\text{-AlF}_3$	AlF_6	3.4	0	-12.5	[139]
$\beta\text{-AlF}_{6-x}(\text{OH})_x$ ($82 \text{ m}^2 \text{ g}^{-1}$)	AlF_6 and $\text{AlF}_5(\text{OH})$	0.28	qp	-15.5	[140]
	$\text{AlF}_4(\text{OH})_2$	0.61	qp	-11.7	[140]
	$\text{AlF}_3(\text{OH})_3$	0.990	qp	-9.5	[140]
HS-AlF_3	site A/B	3.88/8.68	qp/qp	4.8/-7.9	[141]
	site C/D	6.37/5.04	qp/qp	-7.4/-7.7	[141]
$\text{H}_3\text{AlF}_6 \cdot 6\text{H}_2\text{O}$	AlF_6	0.3	0.0	-2.8	[142]
$\text{K}_2\text{AlF}_5 \cdot \text{H}_2\text{O}$	AlF_6	12	0.0	0	[142]
RbAlO_2	5 sites	2.7-8.7	0.03-0.65	20.5-69.9	[143]
$\text{Rb}_2\text{Al}_2\text{O}_2\text{F}_2$	AlO_4	9.7	0.00	67.8	[143]
RbAlF_4	AlF_6	13	0.1	-4	[142]
$\text{Rb}_2\text{AlF}_5 \cdot \text{H}_2\text{O}$	AlF_6	13	0.0	0	[142]
$\text{CsAlF}_5 \cdot \text{H}_2\text{O}$	AlF_6	7.5	0.15	-10	[142]
NH_4AlF_4	AlF_6	10	0.1	-6	[142]
KAlF_4	AlF_6	12	0.0	-5	[142]
	AlF_6	-	-	-19.5	[144]
K_3AlF_6	AlF_6	-	-	-1.2	[144]

Tl ₂ AlF ₅	AlF ₆	-	-	-0.8	[144]
α-BaAlF ₅	AlF ₆	-	-	-13.4	[144]
β-Ba ₃ AlF ₉	3 sites	0.14-0.51	0.07-0.85	-2-1	[145]
Ba ₃ Al ₂ F ₁₂	AlF ₆	-	-	-11.7	[144]
β-CaAlF ₅		1.53	0.10	-	[146]
Al ₁₃ Si ₅ O ₂₀ (OH,F) ₁₈ Cl (zunyite)	Al1 _{Keggin}	2.25	1.0	72.2	[147]
	Al1 _{Pentamer}	1.96	0.7	46.5	[147]
	Al2 _{without F}	2.80	0.4	7.8	[147]
	Al2 _{with one F}	7.08	0.4	14.0	[147]
Al ₂ SiO ₄ F ₂ (topas)	AlF ₆	1.7	0.4	0.3	[142]
Na ₃ AlF ₆ (cryolite)	AlF ₆	0.58	0.89	-0.5	[148]
	AlF ₆	0.600	0.9	-	[138]
	AlF ₆			-0.8	[144]
	AlF ₆	2.0	0	1.4	[139]
K ₂ NaAlF ₆ (elpasolite)	AlF ₆	1.4	0	0.8	[139]
Na ₅ Al ₃ F ₁₄	AlF ₆ 1/2	8.2/6.5	0/1	-1/-3	[139]
Na ₂ MgAlF ₇ (weberite)	AlF ₆	2.15	0.56	-5.4	[148]
Na ₃ Al ₂ Li ₃ F ₁₂ (cryolithionite)	AlF ₆	1.03	0.09	-0.5	[148]
Na ₅ Al ₃ F ₁₄ (chiolite)	AlF ₆	8.0	0.13	-2.5	[148]
	AlF ₆ 1/2	5.867/8.000	0.0/0.1	-	[138]
Na ₂ Ca ₃ Al ₂ F ₁₄	AlF ₆	0.433	0	-1.6	[149]
α-NaCaAlF ₆	AlF ₆ (i)/(ii)	3.800/2.933	0.25/0.1	-3.4/-2.2	[149]
β-NaCaAlF ₆	AlF ₆ (i)/(ii)	1.300/0.400	0/0	-3/-3	[149]
60 NaPO ₃ 40AlF ₃ glass	Al ⁽⁶⁾ / Al ⁽⁵⁾ / Al ⁽⁴⁾	5.1/6.0/3.3	-	-4.5/19/44	[129]

Nitrogen containing materials

AlO_{4-x}N_x (AlON) and (Si, Al)_x(O, N)_{x+1} (SiAlON) materials, see [150], for ceramic [151]

SiAlON	AlO ₆	-	-	2.8	[152]
γ-AlON	AlO ₆	-	-	14	[153]
SiAlON	AlO ₄	-	-	59	[152]
γ-AlON	AlO ₄	-	-	66	[153]
AlON or Al ₂ O ₃ /AlN composite	AlNO ₃	-	-	96	[153]
AlON or Al ₂ O ₃ /AlN composite	AlN ₂ O ₂	-	-	96	[153]
AlON or Al ₂ O ₃ /AlN composite	AlN ₃ O	-	-	106	[153]
AlN	AlN ₄	-	-	114-117	[153]
Li _{0.06} Al _{2.72} O _{3.77} N _{0.23} (LiAlON)	AlO ₆	4.83	0.61	15.35	[154]
	AlO ₅ N	7.77	0.61	16.89	[154]
	AlO ₄	3.79	0.61	67.02	[154]
	AlO ₃ N	6.83	0.61	72.00	[154]
CaMg ₂ AlN ₃	AlN ₄	5.6	-	120	[155]

Other aluminum compounds

Al ₄ C ₃	Al1	15.58	0	120.1	[156]
	Al2	15.83	0	111.2	[156]
Al ₄ C ₃ (Strem/Zegen)	site 1	16.5/16.7	0.0/0.0	119.9/119.6	[157]
	Site 2	14.1/14.5	0.1/0.1	109.4/109.1	[157]
	AlOC-1	109.0/10.7		104/100.2	[157]
	AlOC-2	-	-	96.3/97	[157]
Al(acac) ₃	AlO ₆	3.03	0.15	0.0	[158]
Al(trop) ₃		4.43	0.08	36.6	[158]
Al(TMHD) ₃	AlO ₆	3.23	0.10	1.5	[158]
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	[159]
[Al ₈ (OH) ₁₄ (H ₂ O) ₁₈](SO ₄) ₅ ·16H ₂ O	3 sites	3.2/5.75/3.10	8/0.1/0.5	4.8/8.4/11.0	[160]

$\text{Al}_2(\text{OH})_2(\text{H}_2\text{O})_8(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$	AlO_6	4.6	0.4	3	[4]
$\text{Al}_2(\text{OH})_4\text{SO}_4 \cdot 7\text{H}_2\text{O}$ (aluminite)	$\text{AlO}_6\text{-}1/2$	10.1/11.6	0.1/0.15	6.9/6.4	[4]
$\text{NaAlCO}_3(\text{OH})_2$ (dawsonite)		6.70	0.45	10	[161]
$\text{Ca}_6\text{Al}_2\text{S}_3\text{H}_{64}\text{O}_{50}$	AlO_6	0.36	0.19	13.1	[30]
$\text{Ca}_4\text{Al}_2\text{SH}_{24}\text{O}_{22}$	AlO_6	1.7	qp	11.8	[30]
$\text{Ca}_4\text{Al}_6\text{O}_{12}\text{SO}_4$ (ye'elimite)	8 sites	2.5-7.6	0.07-0.76	73.6-76.1	[162]
$\text{Ca}_6[\text{Al}(\text{OH})_6]_2(\text{SO}_4)_3 \cdot 26\text{H}_2\text{O}$ (ettringite)	Al(1)	0.391	0.164	13.08	[163]
	Al(2)	0.337	0.174	13.51	[163]
$\text{Ca}_4[\text{Al}(\text{OH})_6]_2(\text{CrO}_4) \cdot 12\text{H}_2\text{O}$	AFm mono	1.10	0.16	11.26	[164]
$\text{Ca}_4[\text{Al}(\text{OH})_6]_2(\text{CrO}_4)_{0.5}(\text{OH}) \cdot 12\text{H}_2\text{O}$	AFm hemi	1.04	0.25	11.26	[164]
$\text{Ca}_6[\text{Al}(\text{OH})_6]_2(\text{CrO}_4)_3 \cdot 24\text{H}_2\text{O}$	Aft Al(1)/Al(2)	0.353/0.359	0.293/0.245	13.05/13.44	[164]
$\text{KAl}_3(\text{SO}_4)_2(\text{OH})_6$ (alunite)	Al1	10.40	0.05	4.7	[165]
	Al ₁₁ / Al ₁₂	-	-	-3.3/0.1	[165]
$\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	AlO_6	0.400	0.00	-4.1	[36]
$\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	AlO_6	0.456	0.00	-0.4	[36]
ZnAl-CO₃ , layered double hydroxides synthesized at different pH					
	Al-1	1.3-1.4	0.67-0.71	15.1-15.2	[166]
	Al-2	3.1-3.3	0.61-0.70	13.4-15.0	[166]
Host compounds					
Ca_2SiO_4 larnite (belite)	Al _{IV}	7.1	0.33	96.1	[167]
	Al _{VI}	4.5	0.4	10.1	[167]
	AlO_4	5.8	0.54	94	[168]
MgO periclase	AlO_6	<0.45	-	15.8	[168]

Table 8.2. ^{23}Na , quadrupole coupling constant $C_Q = e^2qQ/h$, the asymmetry parameter η , and the isotropic value of the chemical shift δ (referred to 1.0 M NaCl [3]) 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 $\delta(\text{referenced to 1M NaCl}) = \delta(\text{referenced to solid NaCl}) + 7.2 \text{ ppm}$. 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 $P_Q = C_Q \sqrt{1 + \frac{\eta^2}{3}}$ 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	[169]
		1.4	0.7	22.1	[170]
		1.46	0.71	22.65*	[171]
$\text{Na}_2\text{SiO}_3 \cdot 9\text{H}_2\text{O}$		1.110	0.63	3.7	[172]
$\text{Na}_2\text{SiO}_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$		1.14	0.56	3.53*	[171]
$\text{Na}_2\text{SiO}_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$	Na 1/2	1.80/2.83	0.75/0.17	9.00*/9.50*	[171]
$\alpha\text{-Na}_2\text{Si}_2\text{O}_5$		1.820	1	17.1	[169]
		1.79	1.0	16.9	[173]
		132.3 MHz	1.82	1	17.1
$\text{Na}_2\text{Si}_2\text{O}_5$, SKS-5, layered, hydrated, site 2		1.6	0.8	0.8	[175]
	site 3/4	0.5/1.2	qp/0.2	-1.0/-0.7	[175]
$\text{Na}_2\text{Si}_2\text{O}_5$, SKS-6, layered, hydrated, site 5/6		1.7/1.6	0.5/0.8	-1.1/0.8	[175]
	site 7/8	1.2/0.6	0.2/ qp	-1.0/-1.0	[175]
$\delta\text{-Na}_2\text{Si}_2\text{O}_5$	Na _b 5 c	2.4	1	10	[169]
	site B	2.4	1.0	8.4	[176]
	(2) 132.3 MHz	2.4	1	9.1	[174]
	Na _c 6 c	1.1	0.3	15.9	[169]
	site A	1.1	0.3	15.4	[176]
	(1) 132.3 MHz	1.16	0.25	16.1	[174]
$\beta\text{-Na}_2\text{Si}_2\text{O}_5$	Na(1)	2.29	0.85	15.6	[173]
	(2) 132.3 MHz	2.5	0	18.7	[174]
	Na(2)	2.20	0.55	9.4	[173]
	(1) 132.3 MHz	2.22	0.55	9.4	[174]
$\text{Na}_2\text{O} \cdot 4\text{SiO}_2 \cdot 5\text{H}_2\text{O}$ (makatite)	site 1/2/3	1.3/1.5/1.4	0.6/0.4/0.6	0/1/8	[177]
$\text{Na}_2\text{O} \cdot 8\text{SiO}_2 \cdot 9\text{H}_2\text{O}$ (octosilicate)		0.48	-	-0.7	[177]
$\text{Na}_2\text{O} \cdot 8\text{SiO}_2 \cdot x\text{H}_2\text{O}$ (octosilicate dried)		2.4	0.7	-6	[177]
$\text{NaSi}_2\text{O}_5 \cdot 3\text{H}_2\text{O}$ (kanemite)	site 1/2/3	1.7/2.0/0.6	0.7/0.7/-	0/2/-1	[177]
$\text{Na}_2\text{Si}_{14}\text{O}_{29} \cdot 11\text{H}_2\text{O}$ (magadiite)		1.3	0.6	0	[177]
$\text{Na}_2\text{Si}_{22}\text{O}_{41}(\text{OH})_8 \cdot 6\text{H}_2\text{O}$ (kenyaite)		0.60	-	-0.5	[177]
$\text{Na}_8\text{Si}_{12}\text{O}_{28} \cdot 4\text{H}_2\text{O}$ (Mu-11)	(A)/ (B)	2.7/2.9	0.4/0.7	1/0.7	[178]
$\text{Na}_2\text{BaSi}_2\text{O}_6$	Na 1/Na 2	2.10/2.96	0.75/0.1	25.0/5.4	[173]
$\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 8\text{H}_2\text{O}$		1.11	0.72	3.8*	[179]
$\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 4\text{H}_2\text{O}$	(1)/(2)	1.80/2.83	0.75/0.17	9.0*/9.5*	[179]
$10\text{Na}_2\text{O} \cdot 10\text{CaO} \cdot 21\text{B}_2\text{O}_3 \cdot 8\text{Al}_2\text{O}_3 \cdot 51\text{SiO}_2$ (glass)		2.8	0.7	-7.9	[180]
$43.1\text{Na}_2\text{O} \cdot 56.9\text{SiO}_2$ (glass)		3.0	-	7.5	[181]
Soda-lime silicate glass		1.9	-	4.7	[182]
$\text{Na}_4\text{Ti}_2\text{Si}_8\text{O}_{22} \cdot 5\text{H}_2\text{O}$ (penkvilksite)		3.30	0.45	4.3	[183]
$\text{Na}_3\text{F} \cdot \text{SnSi}_3\text{O}_9$ (stannosilicate)	(A)/ (B)	3.0/3.7	0.55/0.68	12.5/9	[184]

Zeolites and zeolite-like materials

Na-A (dehydrated) near to 6- rings	5.8	0	-	[185]	
near to 4, 8-rings	3.2	0.9	-	[185]	
Na-LSX (93.2 Na/u.c.)	SI	1.2	0.1	0	[186]
(dehydrated)	SI'	5.9	0.1	-6	[186]
	SII	5.1	0.2	-12	[186]
	SIII'(1,2)	2.2	0.5	-13	[186]
	SIII'(3)	2.0	0.8	-1	[186]
Na-LSX (dehydrated)	SI	1.1	0.5	5.2*	[187]
	SI'	5.8	0.0	-12.8*	[187]
	SII	5.0	0.0	-8.8*	[187]
	SIII'(1,2)	2.2	0.7	-10.8*	[187]
	SIII'(3)	1.2	0.9	-22.8*	[187]
39Li86NaLSX (dehyd.)	SI	1.1	0.5	5.2*	[187]
	SI'	5.4	0.0	-11.8*	[187]
	SII	4.8	0.1	-8.8*	[187]
	SIII'	0	-	-21.8*	[187]
84Li16NaX (dehydr.)	SIII'	0	-	-22.8*	[187]
Na-X (83.5 Na/u.c.)	SI	1.2	0.1	-1	[186]
(dehydrated)	SI'	5.9	0.1	-10	[186]
	SII	4.8	0.2	-16	[186]
	SIII'(1,2)	2.6	0.5	-17	[186]
	SIII'(3)	2.0	0.8	-11	[186]
Na-X (Si/Al=1.23) MAS/DOR	SI	0/-	0/-	1.2/-*	[188]
(dehydrated)	SI'(1)	5.2/5.0	0/0	-11.8/-12.8*	[188]
	SI'(2)	-/3.6	-/0	-/-20.8*	[188]
	SII	4.6/4.5	0/0.1	-7.8/-10.8*	[188]
	SIII'(1,2)	2.6/3.0	0.7/0.5	-5.8/-3.8*	[188]
	SIII'(3)	1.6/1.9	0.9/0.9	-21.8/-23.8*	[188]
Zeolite Na-X (Si/Al=1.24)	SI	1.4	0	-2.7	[189]
(dehydrated)	SI'	5.4	0	-20	[189]
	SII	4.9	0	-10	[189]
	SIII'(1,2)	3.0	0.5	-11	[189]
	SIII'(3)	2.1	0.9	-21	[189]
Na-Y (Si/Al=2.5) (dehydrated)	SI	0	0	-4.8*	[188]
Na-Y (Si/Al=2.6) (dehydrated)	SI	1.2	qp	-5	[190]
	SI	1.2	0	-1.5	[189]
	SI'	4.8	0	-12	[189]
	SII	3.9	0	-8	[189]
Na-Y (Si/Al=2.7) (dehydrated)	SI	1.2	0.5 _{assumed}	-3.3*	[191]
	SI'	2.6	0.5 _{assumed}	-5.4*	[191]
	SII	3.8	0.5 _{assumed}	-13.0*	[191]
Na-Y (Si/Al=8.6) (dehydrated)	two SI sites	1.1/1.2	0.5 _{assumed}	-1.2/-6.1*	[191]
	in sodalite c.	1.6	0.5 _{assumed}	-18.1*	[191]
	SII	3.5	0.5 _{assumed}	-11.7*	[191]
Na-Y (Si/Al=2.56) (dehydrated)	SI	0.4	qp	-6	[192]
	SI'/SII'	2.3	qp	-12	[192]
	SII	4.2	qp	-4	[192]
	SIII	4.7	qp	5	[192]
Na-Y (Si/Al=2.6) (dehydrated)	SI	1.2	0.1	-3	[186]
	SI'	4.8	0.2	5	[186]
	SII	3.9	0.2	-7	[186]

HNa-Y (21.3 Na/u.c.) (dehyd.)	SI	1.2	0.1	-3	[186]
	SI'	4.9	0.2	5	[186]
	SII	3.8	0.2	-7	[186]
HNa-Y (13.3 Na/u.c.) (dehydr.)	SI	1.2	0.1	-3	[186]
	SI'	4.9	0.3	5	[186]
	SII	3.8	0.2	-7	[186]
HNa-Y (2.7 Na/u.c.) (dehydr.)	SI	1.2	0.1	-3	[186]
	SI'	4.8	0	3.2*	[188]
	SII	3.9	0	-4.8*	[188]
Ca ₁₉ Na ₁₆ -Y (Si/Al=2.56) (dehy.)	SI	0.4	qp	-2	[192]
	SI'/SII'	2.3	qp	-4	[192]
	SII	4.6	qp	-3	[192]
	SIII	5.0	qp	3	[192]
75Na25K CHA (dehydr.)	SIIa	5.7	qp	-8.1*	[193]
	SIII'a	4.1	qp	-17.5*	[193]
	SIII'b	1.7	qp	-2.8 to -15.6*	[193]
31Li47Na22K CHA (dehy.)	SI	1.2	qp	6.2*	[193]
	SIIa	4.9	qp	-6.8*	[193]
	SIIb	5.3	qp	-4.8*	[193]
	SIII'a	4.1	qp	-17.8*	[193]
	SIII'b	2.0	qp	-3.8 to -13.1*	[193]
	SIII'a	4.4	qp	-15.8*	[193]
Na-EMT (Si/Al=3.7) (dehydr.)	SI	1.0	qp	-6.5	[190]
Na-MOR (Si/Al=7.1) (dehydr.)	12-ring	2.0	qp	-14	[190]
	sidepockets	3.1	qp	-24	[190]
Na-MOR (Si/Al=6.49) (dehydr. 773 K) (18.8 T)					
	Na VI	2.3	0.56	-12.4	[194]
	Na IV	2.9	0.46	-19.2	[194]
	Na I	2.9	0.56	-24	[194]
Na-FER (Si/Al=27)	Na I	4.3	0.6	-1.5	[195]
	Na IIa	2.2	0.6	-15.5	[195]
	Na IIb	2.1	0.6	-19.5	[195]
	Na III	3.6	0.6	-22.5	[195]
Na-ZSM-5 (Si/Al=18) (dehydr.)	10-ring	2.0	qp	-18	[190]
SSZ-13 zeolite (Si/Al=21)	SIIa0/SIIa1	3.1/3.9	0.6/0.2	-11.2/-7.4	[196]
	SIII'a1/SIII'b	2.7/1.8	1/0.6	-20.4/-10.0	[196]
K,Na-JBW (Na ₂ Rb-[AlGeO ₄] ₃ ·H ₂ O)		1.8	1.1	5	[92]
Na ₂ Al ₂ Si ₃ O ₁₀ ·2H ₂ O (natrolite)		1.82	0.6	8.18	[197]
NaAlSi ₃ O ₈ (albite)		2.69	0.25	-7.1	[198]
NaAlSi ₂ O ₆		3.3	0.25	11.0	[173]
Na,K AlSi ₃ O ₈ (feldspar)	8 samples	2.136-1.160	0.6-0.7	-20.1--24.7	[120]
Na ₈ Al ₂ Be ₂ Si ₈ O ₂₄ Cl ₂ (tugtupide)		1.41	0.44	7.7	[117]
Na(Na ₂)Mg ₅ Si ₈ O ₂₂ (OH) ₂ OH	M(4)	3.9	0.49	9.3	[122]
(HSMC) channel (A)		2.9	0.26	5.5	[122]
Na _{8.0} [AlSiO ₄] ₆ Cl _{1.8} ·0.4 H ₂ O (NaCl-sodalite)		0.20-0.45	qp	-8.8	[95]
Na _{7.7} [AlSiO ₄] ₆ Br _{1.8} ·0.4 H ₂ O (NaBr-sodalite)		0.72	0.12	-9.9	[95]
Na _{7.8} [AlSiO ₄] ₆ I _{1.7} ·0.4 H ₂ O (NaI-sodalite)		1.73	0.06	-20.6	[95]
Na ₈ Cl ₂ [Al ₆ Si ₆ O ₁₂] (NaCl-sodalite)		≈0	0.67 _{assumed}	6.3	[199]
Na ₈ B ₂ [Al ₆ Si ₆ O ₁₂] (NaB-sodalite)		1	0.67 _{assumed}	8.5	[199]
Na ₈ I ₂ [Al ₆ Si ₆ O ₁₂] (NaI-sodalite)		1.9	0.67 _{assumed}	9.3	[199]
Na ₈ Cl ₂ [Al ₆ Si ₆ O ₂₄] (NaCl-sodalite)		0.5	qp	6.1	[93]
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄] (NaBr-sodalite)		0.7	qp	7.2	[93]

Na ₈ I ₂ [Al ₆ Si ₆ O ₂₄] (NaI-sodalite)	1.8	qp	7.3	[93]	
Na ₈ [Al ₆ Si ₆ O ₂₄]·(H ₃ O ₂) ₂ (basic sodalite)	0.8	qp	5	[96]	
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄] · (basic sodalite)	0.7	qp	7.5	[96]	
Na ₆ [Al ₆ Si ₆ O ₂₄]·(4H ₂ O) ₂ (hydro sodalite)	1.1	qp	-0.1	[96]	
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄]	0.7	qp	7.4	[96]	
Na ₆ [Al ₆ Si ₆ O ₂₄] (dry sodalite)	5.6	qp	-	[96]	
Na ₈ Br ₂ [Al ₆ Si ₆ O ₂₄] (dry sodalite)	0.7	qp	7.4	[96]	
Na ₆ [AlSiO ₄] ₆ (anhydrous sodium sodalite)	5.90	0.10	10.2*	[171]	
Na ₈ [AlSiO ₄] ₆ (OH) ₂ (hydroxosodalite, dehyd.)	2.00	0.10	3.2*	[171]	
Na ₈ [AlSiO ₄] ₆ (OH) ₂ ·2H ₂ O (hydroxosodalite)	1.55	0.16	-1.2*	[171]	
Na-nitride sodalite	1.00	0.18	0.4*	[179]	
Na ₈ Cl ₂ (AlSiO ₄) ₆ (blue sodalite)	0.081	0.35	95 ?	[94]	
Na ₈ Si ₁₂ O ₂₈ ·4H ₂ O (Mu-11)	(A)	2.7	0.4	1	[178]
	(B)	2.9	0.7	0.7	[178]
Na ₆ Zn ₂ [AlSiO ₄] ₆ (SO ₄) ₂	1.9	qp	1	[98]	
NaAlSi ₂ O ₆ (jadeite)	3.30	0.25	11.0	[173]	
(Na ₄ BH ₄) ³⁺ sodalite	AlSi	8.82	0	-6.61	[200]
	GaSi	6.41	0	-1.31	[200]
	AlGe	6.75	0.22	-1.60	[200]

Other (non-zeolite) aluminosilicates

Al ₂ O ₃ -B ₂ O ₃ -SiO ₂ -Na ₂ O glasses	2.5-3.5	qp	-3--12	[100]	
Soda-lime aluminosilicate glass	1.8	-	-6.9	[182]	
[Na ₂ O·Li ₂ O] _{0.46} [0.16Al ₂ O ₃ ·0.84P ₂ O ₅] _{0.54} glass					
	Al(OP) ₆	2.4-2.6	qp	-10--11	[201]
	Al(OP) ₅	3.3-4.0	qp	16-18	[201]
	Al(OP) ₄	3.4-4.2	qp	46-49	[201]

Nitrogen containing materials

NaNO ₃	-	-	-7.3	[202]
	0.337	0.00	-8.0	[36]
NaNO ₂	1.09	0.11	-0.1	[36]
NaN ₃	-	-	-3.5	[202]
	0.297	0.12	-3.8	[36]

Other (non-zeolite) phosphorus containing materials

Na ₃ P ₃ O ₉	Na 1/Na 2	2.20/1.57	0.70/0.55	-7.60*/1.60*	[171]
NaPO ₃ glass		2.3	-	-4.2	[129]
60 NaPO ₃ 40AlF ₃ glass		2.2	-	-7.3	[129]
Na ₅ P ₃ O ₁₀ H ₂ O	1/2	1.74/1.97	0.29/0.85	-0.55/-5.71	[203]
	3/4	2.09/2.40	0.81/0.51	-9.09/2.20	[203]
	5	1.69	0.26	-4.20	[203]
Na ₅ P ₃ O ₁₀	Na 1/ Na 2	4.65/3.06	0.40/0.17		[204]
	Na 3	4.65	0.40		[204]
Na ₂ P ₂ O ₇ H ₂ O	Na 1/ Na 2	1.37/0.48	0.92/0.99	-	[204]
Na ₄ P ₂ O ₇	Na 1/ Na 2	2.08/2.30	0.26/0.70	5.52/1.96	[205]
	Na 3/ Na 4	2.90/3.22	0.47/0.56	10.41/6.36	[205]
Na ₄ P ₂ O ₇ 10H ₂ O		-	-	1.5	[202]
Na ₃ HP ₂ O ₇ H ₂ O	Na 1/ Na 2	2.55/3.60	0.15/0.20	4.0/1.0	[205]
	Na 3	3.1	0.1	6.5	[205]
Na ₂ HPO ₄	Na 1/ Na 2	0.210/0.325	0.18/0.7	-1.4/-2.5	[206]
	Na 3	0.589	0.26	-1.1	[206]

NaH ₂ PO ₄ ·2H ₂ O		1.19	0.46	2.40*	[171]
NaH ₂ PO ₄ ·H ₂ O		1.22	0.26	-3.49*	[171]
NaH ₂ PO ₄	Na 1/ Na 2	1.59/2.35	0.46/0.94	-	[204]
CaNa ₄ (P ₃ O ₉) ₂	50%/50%	1.405/2.191	0.60/0.69	-3.3/-13.3	[207]
NaMg(PO ₃) ₃	43%/26%	2.67/2.57	0.34/0.47	0.0/-4.3	[208]
	31%	2.72	0.59	-9.8	[208]
NaZn(PO ₃) ₃	41%/28%	2.50/2.66	0.38/0.51	0.0/-4.1	[208]
	31%	2.67	0.59	-9.9	[208]
NaCa(PO ₃) ₃	93%/7%	2.15/0.62	0.88/0.99	3.73/-5.58	[209]
NaSr(PO ₃) ₃		2.38	0.70	2.74	[209]
NaPO ₃ glass		2.1	qp	-3.4	[210]
NaPO ₃ glass		2.52	qp	-5.1	[211]
Na _{0.2} Li _{0.8} PO ₃ glass		2.65	qp	-7.0	[211]
Na _{0.2} Ag _{0.8} PO ₃ glass		2.41	qp	-5.5	[211]
Na _{0.22} K _{0.78} PO ₃ glass		2.34	qp	-1.0	[211]
Na _{0.22} Rb _{0.78} PO ₃ glass		1.93	qp	-0.6	[211]
Na _{0.19} Cs _{0.81} PO ₃ glass		2.52	qp	-1.7	[211]
Na _{0.2} Li _{0.8} PO ₃ glass		2.65	qp	-7.0	[211]
NaPO ₃ -WO ₃ glass		2.0	qp	-14.9	[210]
NaPO ₃ -GeO ₂ glass		1.8	qp	-4.5	[212]
(M ₂ O) _{1/3} [(Ge ₂ O ₄) _x (P ₂ O ₅) _{1-x}] _{2/3} glass		1.3/1.7/1.6	qp	-5.7/-8.3/-4.0	[213]
	M = Na, K x = 0.0, 0.4, 0.8				
60NaPO ₃ -40MoO ₃ glass		2.0	qp	-14.3	[214]
NaGe ₂ (PO ₄) ₃	site 1/2/3	3.45/3.2/-	0.01/0.02/-	-11.5/-21.7/-37.4	[215]
Na _{1.4} Al _{0.4} Ti _{1.6} (PO ₄) ₃		1.4614	-	-8.3	[216]
Na _{1.4} Al _{0.4} Zr _{1.6} (PO ₄) ₃		1.1200	-	-14.6	[216]
Ca ₁₀ K _{0.5} Na _{0.5} (PO ₄) ₇		2.4	0.13	-8.8	[217]
NaSn ₂ (PO ₄) ₃	Na 1/Na 2	2.3/2.5	0/0	-	[218]
Na ₃ Fe ₃ (PO ₄) ₄ (layered)	Na 1/Na 2	1.55/1.57	0.03/0.48	277.5/143.0	[219]
[Na ₂ O·Li ₂ O] _{0.46} [0.16Al ₂ O ₃ ·0.84P ₂ O ₅] _{0.54} glass		1.3	qp	-6	[201]
Ca ₁₀ K _{0.5} Na _{0.5} (PO ₄) ₇		2.4	0.13	-8.8	[217]
Ca ₁₀ Na(PO ₄) ₇		2.48	0.2	-5	[220]
Na ₃ MnPO ₄ CO ₃ (sidorenkite)	1/2	1.2/4.4	0.0/0.5	-168/569	[221]
Na ₆ [P ₂ Mo ₅ O ₂₃]·7H ₂ O	Na(a)/ Na(d)	3.15/2.49	qp/ qp	-1.6/-11.0	[222]
	Na(f)	0.88	qp	-2.1	[222]
HNaPW (hydrated)	1/2	2.0/2.7	1.0/0.0	3/4	[223]
Na ₁₅ [(PO ₂) ₃ PNb ₉ O ₃₄]·22H ₂ O	5 sites	0.63-2.2	0-1	-8.4-3.1	[224]
Na ₅ B ₂ P ₃ O ₁₃	5 sites	1.54-2.83	0.02-0.85	-7.7-9.2	[225]
Others					
Na ₄ Si ₄ (2 at% P-doped)	Na-Si	1.25	1.0	56.7	[226]
	Na-Si	2.31	0.15	49.5	[226]
	Na-P	2.0	0.1	53.3	[226]
Cs ₇ NaSi ₈		5.36	0	72.2	[227]
Rb ₇ NaSi ₈		5.66	0	157.2	[227]
Na ₂ O		≈0	-	55.1	[228]
Na ₂ O ₂	2 sites	-	-	4.8 and 9.9	[229]
Na ₃ OCl		11.34	0.0	-	[228]
NaOH	5-coord.	3.59	0.07	21.1	[230]
		3.5	0.00	19.4*	[171]
NaOH·2H ₂ O		2.20	0.70	12.2*	[171]
NaZrO ₃	Na 1/ Na 2	2.52/2.08	0.67/0.05	15.0/27.0	[231]

	Na 3	4.20	0.27	19.5	[231]
Na ₂ ZrSi ₂ O ₇ (parakeldyshite)	Na 1/Na 2	1.5/2.8	1.0/0.85	0.0/2.0	[232]
Na ₂ ZrSi ₄ O ₁₁ (vlasovite)	Na 1/Na 2	1.65/4.70	0.25/0.0	-4.5/-3.0	[232]
NaZrSi ₆ O ₁₅ ·3H ₂ O (elpidite)	Na 1/Na 2	2.05/2.65	0.50/0.75	-7.0/-1.0	[232]
Na ₄ Zr ₂ Si ₃ O ₁₂	Na 1/Na 2	2.30/3.10	0.85/0.30	-7.0/9.0	[232]
Na ₃ GaF ₆		1.49	0.4	0.1	[233]
NaF		-	-	7.9	[202]
	octahedr.	≈0	-	7.2	[230]
NaCl		-	-	7.9	[202]
	octahedr.	≈0	-	7.2	[230]
NaBr		-	-	6.0	[202]
	octahedr.	≈0	-	5.1	[230]
NaI				-2.7	[202]
	octahedr.	≈0	-	-3.2	[230]
NaIO ₄		-	-	-12.5	[202]
Na ₂ S	tedrahedr.	≈0	-	49.7	[230]
Na ₂ S	site 1	0	-	49.8	[234]
β-Na ₂ S ₂	site 1/site2	≈0/≈0	-/-	8.5/5.9	[234]
Na ₂ S ₄	site 1/site2	1.03/1.71	0.9/0.7	8.9/3.1	[234]
α-Na ₂ S ₅	site 1/site2	1.87/1.52	0.5/0.3	10.5/0.8	[234]
α-NaVO ₃	Na 1/ Na 2	1.5/0.765	0.58/0.06	-15.5/-4.8	[235]
β-NaVO ₃		1.42	0.27	-10.3	[235]
Na ₂ SO ₄		2.60	0.58	-1.3*	[171]
Na ₂ SO ₃	Na 1/ Na 2	1.06/0.33	0.00/0.00	-	[204]
	Na 3	1.14	0.00	-	[204]
NaAlO ₂		2.15	0.60	26.2*	[171]
Na[Al(OH) ₄]		3.10	0.00	5.9	[236]
NaAl ₉ O ₁₄	1/2	2.15/2.65	0.4/0.2	-15.6/-14.6	[38]
Na ₂ Al ₂ B ₂ O	Na 1/Na 2	1.9/0.33	0.1/0	5.5/-7.1	[134]
Na ₂ B ₂₉	50%/50%	2.4/2.2	qp/ qp	10.2/16.9	[237]
NaBO ₂		1.19	0.24	2.1	[135]
		1.2	0.09	1.8	[238]
Na ₄ B ₂ O ₅	Na 1/Na 2	2.2/3.0	1.0/0.5	19.6/14.4	[238]
Na ₂ O·4B ₂ O ₃	Na 1/Na 2	4.1/2.0	0.18/0.35	3.4/ -11.4	[238]
NaBO ₂ ·2H ₂ O		1.530	0.80	10.6	[172]
Na ₂ B ₄ O ₇	62%/20%	2.65/1.8	0.91/0.9	-9.9/-12.0	[135]
	18%	1.8	0.1	-4.9	[135]
Na ₂ B ₄ O ₇ ·10H ₂ O (borax)	Na 1/Na 2	0.541/0.849	0.499/0.143	-	[239]
Na ₂ B ₄ O ₇ ·5H ₂ O (tincalconite)	Na 1/Na 2	0.539/0.785	0.741/0.0	-	[239]
	Na 3	1.299	0.0	-	[239]
NaCa[B ₅ O ₆ (OH) ₆]·5H ₂ O (ulexite)		0.07	-	7.1	[240]
H ₁₅ [Na ₄ (V ₁₂ B ₃₂ O ₈₄)]13H ₂ O (polyoxovanadate)	4 sites	0.5-1.8	0.5	-6-15	[241]
NaSnO ₃ ·3H ₂ O		1.760	0.00	12.8	[172]
NaTeO ₄ ·2H ₂ O		2.240	0.37	12.5	[172]
Na ₂ Te ₄ O ₉	Na 5/Na6	4.4/3.6	0.08/0.12	-3/5	[242]
Na ₂ TeO ₃	Na 1/Na2	1.84/1.36	0.08/0-12	5.8/17.0	[242]
NaNbO ₃ (polar phase)	Na 1/ Na 2	2.4/1.2	qp/ qp	1.5/-5.1	[243]
NaNbO ₃ (perovskite)	MAS	1.3	0.9	-3.0	[244]
Li _{0.05} Na _{0.95} NbO ₃	Na 1/ Na 2	1.1/2.3	qp/ qp	-4.6/-0.6	[245]
NaNbWO ₆	19%/81%	0.4/1.4	0.5/-	-6.5/-18	[246]
NaTaO ₃ (perovskite)	Na 1/Na 2	2.1/1.0	0.0/0.9	-0.5/-4.5	[244]
Na ₂ CrO ₄	Na 1/Na 2	2.78/0.5	0.57/ qp	-12.8*/-6.7*	[171]

NaClO ₄	-	-	-20.4	[202]
	0.80	0.35	-18.3*	[171]
NaClO ₄ ·H ₂ O	Na 1/Na 2	1.71/1.48	0.20/0.10	-4.5*/-5.2* [171]
Na _{1-x} Ge _{3+z} (Na _{0.72} Ge _{3.13})	Na6	-	-	20.5 [247]
	Na5(1)/(2)	0.473/0.414	0.25/0.23	4.5/2.4 [247]
Na ₂ Ge ₂ O ₅		2.3	1.0	14.5 [248]
32Na ₂ O·68GeO ₂ (glass)		3.2	qp	7.9 [248]
14Na ₂ O·86GeO ₂ (glass)		2.5	qp	-4.1 [249]
Na ₂ GeO ₃		1.3	0.8	22.6 [238]
Na ₄ Ge ₉ O ₂₀		2.7	0.54	-2.1 [238]
Na ₂ Ge ₄ O ₉		2.4	0.7	-6.4 [238]
Na ₂ MoO ₄		2.59	0.00	3.2 [250]
Na ₂ MoO ₄ ·2H ₂ O	Na(1) octah.	0.875	0.23	-1.4 [250]
	Na(2) trig.	2.68	0.08	4.0 [250]
60NaPO ₃ -40MoO ₃ (glass)		2.0	qp	-14.3 [214]
Na ₃ UO ₄	site A/B/C	3.4/4.0/2.5	qp	47/18/13 [251]
	site D/E/F	2.6/2.2/2.4	qp	2/-2/-16 [251]
NaUO ₃		1.7	0.5	-29.2 [252]
Na ₄ UO ₅		3.2	0.2	15.1 [252]
Na ₂ U ₂ O ₇	1/2	1.4/2.0	qp/ qp	-19/-14.1 [252]
Na ₂ WO ₄		2.49	0.00	4.5 [250]
Na ₂ WO ₄ ·2H ₂ O	Na(1) octah.	0.88	0.35	-0.9 [250]
	Na(2) trig.	2.7	0.09	6.3 [250]
Na ₂ WO ₄	(A)	5.2	0.0	-4.0 [253]
	(B)/(C)	small/ small	-	-6/-14 [253]
[Na ₂ S] _{2/3} [(B ₂ S ₃) _{1/2} (P ₂ S ₅) _{1/2}] _{1/3} (glass)		1.6	qp	3.8 [254]
Na ₃ AlF ₆ (cryolite)	CN 6	0.83	0.62	2.6 [148]
	Na1	0.840	0.6	2 [138]
	CN 8 site 1	1.43	0.27	-8.4 [148]
	Na2	1.430	0.3	-9 [138]
Na ₅ Al ₃ F ₁₄ (chiolite)	Na1/ Na2	1.480/3.180	0.0/0.1	-24/-9 [138]
Na ₂ MgAlF ₇ (weberite)	CN 8 site 1/2	2.48/3.24	0.08/0.26	-28.6/-10.4 [148]
Na ₂ Ca ₃ Al ₂ F ₁₄		3.360	0	5.2 [149]
α-NaCaAlF ₆	(i)/ (ii)	2.340/1.360	0.25/0.1	2.0/-1.6 [149]
β-NaCaAlF ₆		1.200	1	7 [149]
NaCoO ₂		3.98	0.02	48 [255]
Na ₃ AlH ₆ doped/non-doped site Na1		0.50/0.49	0.6/0.7	23.5/23.3 [53]
Na ₃ AlH ₆ doped/non-doped site Na2		0.93/0.93	0.4/0.4	-8.8/-8.9 [53]
Na ₂ LiAlH ₆		<0.1	-	-17.9 [53]
NaAlH ₄		0.15	0.2	-9.2 [53]
NaH		<0.1	-	18.2 [53]
NaHCO ₃				-5.4 [202]
20Na ₂ CO ₃ 80γ-Al ₂ O ₃	Na1/Na2/Na3	1.24/2.12/2.45	qp	5.12/0.12/-6,00 [256]
NaAlCO ₃ (OH) ₂ (dawsonite)		3.64	0.56	2 [161]
Na ₂ C ₂ O ₄		2.43	0.75	- [204]
Na ₃ C ₆₀		3.3	0.08	17.2 [257]

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 [3]) for the ^{17}O NMR of inorganic powder compounds at ambient temperature. For organic compounds, we refer to Wu [258]. Paramagnetic systems such as battery materials are not included. The latter in particular have recently been successfully investigated using ^{17}O NMR, see Grey and coworkers [259, 260]. The last reviews concerning solid-state ^{17}O NMR investigations of inorganic material were presented by Asbrook *et al.* [261], Asbrook and Smith [262], and Gerothanassis [263]. First natural abundance ^{17}O NMR spectra of diamagnetic MOFs were presented by Carnevale *et al.* [264]. The data in the table, which were published in the years 1989-2000, were compiled by Pingel [265]. 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	[266]
	OAl ₄	1.15	0.13	70.0	[36]
	Al ₂ OH	5.0	0.5	40	[266]
Al(OH) ₃ (bayerite)	Al ₂ OH	6.0	0.3	40	[266]
α -Al ₂ O ₃ (corundum)	OAl ₄	2.17	0.55	75	[266]
	OAl ₄	2.13	0.50	72	[14]
	OAl ₄	< 2.4	-	66	[267]
γ -Al ₂ O ₃ nanoparticles	AlOH	6.1	0.42	39	[268]
	OAl ₃	2.6	0.32	56	[268]
	OAl ₄ surface	1.3	0.35	72	[268]
	OAl ₄ subsurf.	1.2	0.22	61	[268]
γ -Al ₂ O ₃	OAl ₄	1.8	qp	73	[266]
	site 1	2.5	-	56.7	[269]
	site 2	0.6	-	68.6	[269]
	site 3	1.1	-	81.0	[269]
	Site A–E			50–80	[270]
	AlO ₄	3.5	qp	77.5	[271]
	AlO ₅	4.5	qp	37.2	[271]
BaO/ γ -Al ₂ O ₃	AlO ₆	4.3	qp	14.0	[271]
	AlO ₄	4.5	qp	77.4	[271]
	AlO ₅	3.1	qp	34.0	[271]
η -Al ₂ O ₃	AlO ₆	4.2	qp	13.7	[271]
	OAl ₄	1.6	qp	73	[266]
	δ -Al ₂ O ₃	OAl ₄	1.6	qp	72
θ -Al ₂ O ₃	OAl ₄	1.2	qp	72	[266]
	OAl ₃	4.0	0.6	79	[266]
Al ₁₃ O ₄₀ cluster	AlOAl	1.2	0	50	[272]
NaAlO ₂	AlOAl	1.81	qp	30.9	[273]
CaAl ₂ O ₄	nb O	≈1.9	qp	≈141	[273]
	8 br O	1.3-1.9	qp	57.3-86.8	[274]
CaAl ₄ O ₇	O1	1.9	0.7	71.6	[274]
	O2 or O3	1.8	0.5	61.5	[274]
	O3 or O2	2.1	0.5	56.8	[274]
	O4	2.5	0.4	40.6	[274]
LaAlO ₃		1.6 (max.)		170.2	[275]
Y ₃ Al ₅ O ₁₂	OY ₂ Al ₂	1.49	0.99	142	[14]
Y ₄ Al ₂ O ₉	9 sites	1.49	qp	126-372	[14]

YAlO ₃	O ₍₁₎ Y ₃ Al ₂	1.57	1.00	143	[14]
	O ₍₂₎ Y ₃ Al ₂	1.65	0.35	165	[14]
Silicates without aluminum					
Siliceous zeolite Y, Sil-Y dehydrated	SiOSi O1	5.1	0.3	42.3	[276]
	SiOSi O2	5.39	0.2	37.2	[276]
	SiOSi O3	5.14	0.1	47.3	[276]
	SiOSi O4	5.28	0.2	34.8	[276]
Siliceous ferrierite, Sil-FER dehydrated	SiOSi 1/2	5.62/5.22	qp	43.1/41.6	[277]
	SiOSi 3/4	5.35/5.29	qp	40.7/39.6	[277]
	SiOSi 5/6	5.38/5.27	qp	39.0/37.0	[277]
	SiOSi 7/8	5.32/5.46	qp	37.0/35.9	[277]
	SiOSi 9/10	5.64/5.57	qp	34.8/28.0	[277]
SiO ₂ (low cristobalite)	SiOSi MAS	5.3	0.0	44	[278]
SiO ₂ (α-cristobalite)	SiOSi	5.3	0.125	36.7	[279]
		5.35	0.21	37.5	[280]
SiO ₂ (α-quartz)	SiOSi	5.21	0.19	43	[280]
SiO ₂ (amorphous)	SiOSi	5.8	0.0	50	[281]
	SiOH	4.0	0.3	20	[281]
	SiOH	4.4	0.0	37	[282]
SiO ₂ (stishovite)	OSi ₃	6.5	0.125	109	[283]
SiO ₂ (coesite)	SiOSi O5	5.16	0.292	58	[284]
	SiOSi O2	5.43	0.166	41	[284]
	SiOSi O3	5.45	0.168	57	[284]
	SiOSi O4	5.52	0.169	53	[284]
	SiOSi O1	6.05	0.000	29	[284]
SiO ₂ (glass)	SiOSi	5.08	0.150	37.58	[285]
2Mg ₂ SiO ₄ ·Mg(OH) ₂ (hydr.-chondrodite)	OH	6.6	0.1	25	[286]
4Mg ₂ SiO ₄ ·Mg(OH) ₂ (hydr.-clinohumite)	OH	7.0	0.2	25	[286]
β-Mg ₂ SiO ₄ (hydr. wadsleyite)	O2	4.9	0.9	76	[287]
		5.0	0.9	78	[288]
	O3	4.4	0.2	66	[287]
	O4	3.8	0.3	65	[287]
	O1	1.3	qp	38	[287]
Mg ₂ SiO ₄ (forsterite)	SiOMg-I	2.35	0.2	61	[289]
		2.8	qp	64	[290]
	O3 3QMAS	2.5	0.2	61	[291]
	SiOMg-II	2.35	1.0	62	[289]
		3.3	qp	72	[290]
	O2 3QMAS	2.5	0.4	64	[291]
	SiOMg-III	2.70	0.3	47	[289]
		3.0	qp	49	[290]
	O1 3QMAS	2.9	0.3	48	[291]
Mg ₃ Si ₄ O ₁₀ (OH) ₂ (talca)	SiOMg	3.2	0.0	40	[281]
	SiOSi	5.8	0.0	50	[281]
	MgOH	7.3	0.0	0	[281]
2Mg ₂ SiO ₄ ·Mg(OH) ₂ (chondrodite)	O1/O2	2.5/2.3	0.3/0.2	63/60	[286]
	O3/ O4	2.3/2.7	0.3/0.2	59/52	[286]
4Mg ₂ SiO ₄ ·Mg(OH) ₂ (clinohumite)	O2/ O6	2.5/2.4	0.3/0.2	65/64	[286]
	O3+O4	2.3	0.1	61	[286]
	O7/ O8	2.4/2.4	0.2/0.2	60/59	[286]
	O5/O1	2.7/2.7	0.2/0.2	52/49	[286]

MgSiO ₃ (ortoenstatite)	O21/ O22	2.8/2.9	qp/ qp	42/46	[292]
	O11/O12	3.0/3.0	qp/ qp	52/54	[292]
	O31/ O32	4.3/4.9	qp/ qp	64/73	[292]
MgSiO ₃ (protoenstatite)	O1+impurity	2.8	qp	52	[292]
	O2/ O3	2.7/4.3	qp/ qp	39/66	[292]
MgSiO ₃ (clinoenstatite)	O21/ O22	2.8/2.8	qp/ qp	45/41	[292]
	O11/ O12	3.0/3.0	qp/ qp	51/54	[292]
	O31/ O32	4.3/4.8	qp/ qp	64/75	[292]
	6 sites	2.9–5.2	qp	57-70	[290]
	SiOMg-I	3.2	0.0	60	[293]
	SiOMg-II	3.2	0.0	42	[293]
	SiOSi	5.1	0.3	62	[293]
Mg ₃ Si ₄ O ₁₀ (OH) ₂ (talc)	SiOMg	3.2	0.0	40	[281]
	SiOSi	5.8	0.0	50	[281]
	MgOH	7.3	0.0	0	[281]
CaMgSi ₂ O ₆ (diopside)	SiOCa	2.7	0.0	84	[293]
	SiOCa	2.83	0.13	86	[290]
	O1 81.4 MHz	2.7	qp	85	[292]
	SiOMg	2.7	0.1	63	[293]
	SiOMg	2.74	0.00	64	[290]
	O2 81.4 MHz	2.9	qp	63	[292]
	SiOSi	4.4	0.3	69	[293]
	SiOSi	4.39	0.36	69	[290]
	O3 81.4 MHz	4.3	qp	70	[292]
	α-CaSiO ₃ (pseudowollastonite)	br O	3.8	0.2	75
	2 nb O	2.3/2.1	0.1/0.1	91/94	[293]
CaSiO ₃ (wollastonite)	9 sites	2.0-4.8	qp	67-115	[290]
Ca ₂ SiO ₄ (larnite)	4 sites	2.5-2.9	qp	122-134	[290]
38.5CaO·61.5SiO ₂ (glass CS46)	nb O	2.1	qp	104.7	[294]
	SiOSi	4.3	qp	62.7	[294]
Li ₂ Si ₂ O ₅	br O1	5.6	0.55	108	[295]
	br O2	4.05	0.05	35	[295]
	nb O3	2.45	0.1	38	[295]
Li ₂ Si ₂ O ₅ (glass)	br O	5.0	0.15	68	[295]
	nb O	2.55	0.2	42	[295]
Na ₂ SiO ₃	br O2	4.20	0.58	63	[170]
	nb O1	2.43	0.17	39	[170]
α-Na ₂ Si ₂ O ₅	br O1/ br O2	5.74/4.67	0.2/0.3	52/74	[295]
	br O1/ br O2	5.7/4.7	0.0/0.25	55/55	[283]
	nb O3	2.4	0.2	36	[295]
		2.35	0.1	34	[283]
ε-Na ₂ Si ₂ O ₅	nb O	-	-	45	[283]
Na ₂ Si ₂ O ₅ (glass)	br O	4.9	0.1	69	[295]
	nb O	2.35	0.2	37	[295]
Na ₂ Si ₄ O ₉ (glass)	SiOSi	5.2	0.22	51	[296]
	nb O	2.7	0.25	40	[296]
	H ₂ O	6.0	0.7	20	[296]
Na ₂ Si ₃ O ₇ (glass)	br O/ nb O	5.0/2.3	0/0	60/39	[283]
24Na ₂ O·76SiO ₂ (glass)	SiOSi	4.73	0.5	48.3	[297]
	SiONa	2.03	0.6	32.2	[297]
	SiOSi	5.1	0	42.6	[298]
Na ₈ Si ₃₂ O ₆₄ (OH)·32H ₂ O (sodium ilerite, RUB-18)	SiOH	3.1	0	61.2	[298]
	SiOZr 1	2.68	0.0	169.5	[232]

	SiOZr 2	2.75	0.1	118.0	[232]
	SiOZr 3	2.80	0.2	126.0	[232]
ZrSiO ₄	SiOZr	-	-	160	[232]
K ₂ Si ₂ O ₅	br O1/O2	5.1/4.7	0.1/0.2	114/69	[295]
	nb O3	2.1	0.5	72	[295]
K ₂ Si ₂ O ₅ (glass)	br O	4.7	0.25	60	[295]
	nb O	2.5	0.45	84	[295]
K ₂ Si ₄ O ₉ (wadeite)	br O1	4.45	0.35	62.5	[283]
	SiOSi O2	4.90	0.2	97	[283]
KHSi ₂ O ₅	br O	4.9	0.1	51	[299]
	nb O	3.5	0.35	60	[299]
K ₂ Si ₄ O ₉ (glass)	br O	4.9	0	52	[283]
	nb O	2.3	0	76	[283]
Rb ₂ Si ₂ O ₅	br O1	4.4	0.1	124	[295]
	br O2	4.7	0.5	59	[295]
	nb O3	1.9	0.5	93	[295]
Cs ₂ Si ₂ O ₅ (glass)	br O	4.55	0.3	68	[295]
	nb O	3.1	0.55	145	[295]
BaSiO ₃	br O	3.7	0.4	87	[293]
	nb O	1.6	0.1	159	[293]
	nb O	2.1	0.1	169	[293]
Ba ₂ TiSi ₂ O ₈ (fresnoite)	SiOTi	-	-	190 (anisotr.)	[300]
	SiOSi	3		0 (anisotr.)	[300]
LiTiOSiO ₄	TiOSi	3.05	0.35	157	[301]
	nb apical OTi ≈0		-	741	[301]
α-SrSiO ₃	br O	4.1	0.4	80	[293]
	nb O	2.2	0.1	105	[293]
	nb O	2.1	0.1	108	[293]
La _{9.33} (SiO ₄) ₆ O ₂ (apatite-type)	O1 or O2	0.266	0.6	165	[302]
	O2 or O1	0.305	0.6	214	[302]
	O3	0.264	0.6	194	[302]
	O4	-	-	600	[302]
Soda-lime borosilicate glass	SiOSi	4.91	0.34	48.1	[297]
	SiOB	5.24	0.45	61.9	[297]
	BOB	5.07	0.46	84.3	[297]
	SiONa	2.60	1	35.2	[297]
	SiO(Ca, Na)	4.91	0.89	70.5	[297]
Cesium borosilicate glass, CBS-2-1.5	br O slice 1	qp=4.2	0.6	52.9	[303]
	br O slice 2	qp=4.5	0.3	60.1	[303]
	br O slice 3	qp=4.5	0.3	67.8	[303]
	br O slice 4	qp=4.5	0.6	77.5	[303]
	nb O site 2	qp=2.3	-	123.7	[303]
Cesium borosilicate glass, CBS-2-1.5	SiOSi	qp=5.1	0.4	44.7	[303]
	SiOB	qp=5.6	0.8	67.6	[303]
	BOB	qp=5.4	0.7	98.5	[303]
Sodium borosilicate glass, NBS-K0.5R0.25	SiOSi	5.13	qp	42.3	[304]
	SiOSi	5.08	qp	43.9	[304]
	SiOSi	5.08	qp	44.2	[304]
Barium borosilicate glass 40BaO 30B ₂ O ₃ 30SiO ₂	nb BaOSi	2.3	qp	158	[305]
	nb BaOB	3.6	qp	197	[305]
Ba Si glass	br O	4.0	0.3	78	[306]
Ba Ca Si glass	br O	4.1	0.3	68	[306]

Ca Si glass	br O	4.7	0.3	59	[306]
	br O	4.6	0.0	66	[282]
	nb O	2.1	0.2	110	[282]
CaTiSiO ₅ (crystalline titanite)	Ti-O-Ti	0.2	≈1	632	[307]
	Si-O-Ti	2.7–3.2	0.1–0.2	166–189	[307]
PbO-SiO ₂ glasses 0.60 ≤ X _{PbO} ≤ 0.71	Si-O-Si	4.4-4.1	0.5 _{assumed}	74.6-80.2	[308]
	Pb-O-Si	2.9	0.5 _{assumed}	150.7-151.7	[308]
	Pb-O-Pb	3.1-3.0	0.5 _{assumed}	287.5-282.6	[308]

Zeolites and zeolite-like materials

Na-A, dehydrated	SiOAl	3.2	0.2	32 MAS	[278]
	SiOAl O1	3.5	qp	43.6 5QMAS	[309]
	SiOAl O2	3.6	qp	31.2 5QMAS	[309]
	SiOAl O3	3.4	qp	40.8 5QMAS	[309]
Na-A, hydrated	SiOAl O1	3.4	0	43.6	[310]
	SiOAl O2	3.4	0	31.0	[310]
	SiOAl O3	3.4	0.25	40.5	[310]
	SiOAl O1	3.4	qp	40.9	[311]
	SiOAl O2	3.6	qp	31.7	[311]
	SiOAl O3	3.4	qp	42.4	[311]
	SiOAl O1	3.5	qp	44 5QMAS	[312]
	SiOAl O2	3.6	qp	31 5QMAS	[312]
	SiOAl O3	3.4	qp	41 5QMAS	[312]
	SiOAl O1	3.5	qp	43.8 5QMAS	[309]
	SiOAl O2	3.6	qp	31.0 5QMAS	[309]
	SiOAl O3	3.4	qp	41.4 5QMAS	[309]
	K-A, dehydrated	SiOAl O1	3.7	qp	31.6 5QMAS
SiOAl O2		3.7	qp	36.3 5QMAS	[309]
SiOAl O3		3.5	qp	47.2 5QMAS	[309]
K-A, hydrated	SiOAl O1	3.5	qp	50.9 5QMAS	[309]
	SiOAl O2	3.9	qp	33.9 5QMAS	[309]
	SiOAl O3	3.7	qp	54.8 5QMAS	[309]
Sr-A, hydrated	SiOAl O1	3.7	qp	60.2 5QMAS	[309]
	SiOAl O2	3.9	qp	38.0 5QMAS	[309]
	SiOAl O3	3.6	qp	48.7 5QMAS	[309]
Tl-A, hydrated	SiOAl O1	3.3	qp	60.7	[311]
	SiOAl O2	3.6	qp	53.4	[311]
	SiOAl O3	3.2	qp	75.5	[311]
Na,K-LSX, hydrated	SiOAl O1	3.3	qp	50.6	[311]
	SiOAl O2	3.3	qp	42.1	[311]
	SiOAl O3	3.4	qp	45.2	[311]
	SiOAl O4	3.6	qp	36.8	[311]
Na-LSX, hydrated	SiOSi	5.0	qp	53 3QMAS	[312]
	SiOAl O1	3.2	0.4	50.3	[310]
	SiOAl O1	3.5	qp	49 5QMAS	[312]
	SiOAl O2	3.3	0.3	41.7	[310]
	SiOAl O2	3.3	qp	37 5QMAS	[312]
	SiOAl O3	3.4	0.3	45.0	[310]
	SiOAl O3	3.4	qp	42 5QMAS	[312]
	SiOAl O4	3.6	0.15	36.9	[310]
Na,K-LSX, dehydrated	SiOAl O1	3.2	qp	42.5	[313]
	SiOAl O2	3.3	qp	37.9	[313]
	SiOAl O3	3.3	qp	38.7	[313]

	SiOAl O4	3.3	qp	33.1	[313]
	SiOAl O1/O2//O3/O4			43.3/36.1/33.3/25.4	[314]
Rb,K-LSX, dehydrated	SiOAl O1/O2//O3/O4			56.4/47.8/44.7/35.8	[314]
Ga-X	SiOGa	4.0	0.3	28	[315]
	SiOSi	5.0	0.0	50	[315]
	SiOSi	4.6	0.1	44 MAS	[278]
Ba, Na-Y, Si/A=2.74, dehydr.	SiOAl	3.4	0.4	40 MAS	[278]
	SiOSi	5.1	0.15	52 MAS	[278]
Na-Y, dealuminated, dehydr.	SiOSi	5.2	0.2	45 MAS	[278]
Na-Y, Si/A=2.74, dehydrated	SiOAl	3.1	0.2	31 MAS	[278]
NH ₄ -Y, Si/A=2.92, dehydr.	SiOAl	3.2	0.2	31 MAS	[278]
	SiOSi	5.0	0.1	48 MAS	[278]
H-Y, dehydrated	OH δ_{1H} =3.7 ppm	6.0	1.0	21	[316]
	OH δ_{1H} =4.4 ppm	6.2	0.9	24	[316]
	SiO2,3,4-Al	3.7	0.2	27.5	[317]
	SiO1Al	3.5	0.3	33.3	[317]
	SiO2,3,4Si	5.3	0.1	44.0	[317]
	SiO1Si	5.1	0.3	50.0	[317]
Na-ZSM-5, hydrated	SiOSi	5.3	0.12	40.0	[318]
	SiOAl	3.5	0.29	30.0	[318]
H-ZSM-5, dehydrated	OH δ_{1H} =4.2 ppm	7.0	0.75	31	[316]
	OH δ_{1H} =4.2 ppm	6.8	0.5	35	[316]
	OH δ_{1H} =4.2 ppm	5.8	0.6	37	[316]
H-ZSM-5, dehydrated	SiOH	-	-	≈5	[319]
	SiOAl	-	-	≈30	[319]
	SiOSi	-	-	≈50	[319]
H-ZSM-5 (dehydrated)	various	3.9–6.5	0.37–0.84	2.8–4.1	[68]
Na ₆ [AlSiO ₄] ₆ ·8H ₂ O (hydrosodalite)	SiOAl	3.4	qp	39.1	[313]
Na ₆ [AlSiO ₄] ₆ (dehydr. hydrosodalite)	SiOAl	4.3	qp	36.3	[313]
Na ₈ [AlSiO ₄] ₆ (OH) ₂ ·2H ₂ O (hydroxosodalite)		3.4	qp	36.0	[313]
Na ₈ [AlSiO ₄] ₆ (OH) ₂ (dehydr. hydroxosodalite)		3.5	qp	39.2	[313]
Ga-sodalite	SiOGa	4.0	0.3	29	[315]
	SiOSi	5.1	0.0	52	[315]
Na-Ba-Ga-sodalite	SiOGa	4.0	0.3	29	[315]
	SiOSi	5.1	0.0	52	[315]
AlPO ₄ -5	AlOP	5.7	0.0	63	[315]
AlPO ₄ -11	AlOP	5.7	0.0	64	[315]
AlPO ₄ -17	AlOP	5.6	0.1	67	[315]
AlPO ₄ -14 as synth., 6 signals	AlOP	4.93–5.85	0.10–0.41	66.8–97.4	[320]
AlPO ₄ -14 calcined, dehydrated	AlOP	5.86	0.16	59.0	[320]
	AlOP	5.76	0.21	68.8	[320]
AlPO ₄ -SIZ-4 (CHA) (EMIMCl)	AlOP O1–O12 (MQMAS)			82–69	[321]
	(DOR)	5.6–5.9	qp	51–78	[321]
AlPO ₄ -SIZ-4 (CHA) (calcined)	AlOP O1	6.38	qp	43.2	[321]
	AlOP O2	6.46	qp	31.8	[321]
	AlOP O3	6.46	qp	33.1	[321]
	AlOP O4	6.33	qp	45.5	[321]
SAPO-34	Al-O-Si	3.5/3.6	0.15/0.10	32/36	[322]
	Al-O-P	6.3/6.1	0.45/0.45	67/74	[322]
Ge-UTL (ADOR parent)	Si-O-Si	5.3	qp	39.3	[323]
ICP-2P (ADOR daughter)	Si-OH			20	[324]
	Si-O-Si			20–40	[324]

MOFs (metal-organic frameworks)

Al MIL-53 (calcined)	Carboxylate	7.1	0.8	230	[325]
	Hydroxyl	5.5	0.7	20	[325]
Al MIL-53 (calcined, hydrated)	Carboxylate1	7.1	0.7	255	[325]
	Carboxylate2	7.9	0.7	225	[325]
	Hydroxyl	7.2	0.9	15	[325]
MIL-53(Al)- <i>np</i>	O1 (μ_2 -OH)	6.37	0.5	25.6	[326]
	O2 (-COO ⁻)	7.77	0.75	228.0	[326]
	O3 (-COO ⁻)	7.36	0.55	235.0	[326]
	O4 (-COO ⁻)	6.95	0.63	258.0	[326]
	O5 (-COO ⁻)	7.57	0.64	264.6	[326]
GaMIL-53 (calcined)	Carboxylate	7.7	qp	230	[325]
	Hydroxyl	4.6	qp	31	[325]
GaMIL-53 (calcined, hydrated)	Carboxylate1	7.5	qp	259	[325]
	Carboxylate2	8.1	qp	230	[325]
	Hydroxyl	5.9	qp	24	[325]
MIL-53 (hydrothermal synthes.)	Al-OH-Al	5.4	0.7	23	[327]
	Al-OH-Ga	4.5	1.0	25	[327]
	Ga-OH-Ga	3.9	1.0	31	[327]
Al-MIL-53 + Ga ₂ (SO ₄) ₃	Al-OH-Al	5.7	0.6	19	[328]
	Al-OH-Ga	4.4	0.9	30	[328]
	Ga-OH-Ga	4.1	0.8	39	[328]
Ga-MIL-53 + Al ₂ (SO ₄) ₃	Al-OH-Al	5.4	0.7	16	[328]
	Al-OH-Ga	4.5	1.0	22	[328]
	Ga-OH-Ga	3.9	1.0	33	[328]
α Mg ₃ (HCOO) ₆ as-made/activated	O1–O12	6.0–7.9	0.2–0.88	227–308	[329]

Other (non-zeolite) aluminosilicates

Na _{0.46} Ca _{2.0} Al _{4.5} Si _{13.5} O ₃₆ · 10.8H ₂ O (stilbite)	SiOSi	5.1	0.18	43	[330]
	SiOAl	3.5	0.28	33	[330]
NaAlSi ₂ O ₆ · H ₂ O (analcime)	SiOSi	5.0	qp	51	[331]
	SiOSi	4.7	qp	51 5Q MAS	[312]
	SiOAl	3.1	qp	35	[331]
	SiOAl	3.2	qp	35 5QMAS	[312]
	AlOAl	1.7	qp	26	[331]
	H ₂ O	6.87	0.67	–15.5	[332]
	H ₂ O	7.6	0	(–?)18	[333]
	Al ₂ Si ₂ O ₅ (OH) ₄ (kaolinite)	SiOSi O3/O4	4.45/4.75	0.43/0.28	54.3/46.5
SiOSi O5		4.65	0.38	51.3	[334]
OH		6.9	0.55	41.5	[334]
SiO2Al		3.4	0.8	6	[334]
KAl ₂ [(OH,F) ₂ /AlSi ₃ O ₁₀] (muscovite)		SiOSi	4.6	0.5	53.0
	SiOSi	4.5	qp	53.2	[335]
	SiO2Al	3.5	0.8	66.5	[334]
	SiO2Al	3.5	qp	66.2	[335]
	SiOAl	3.1	0.5	46.2	[334]
	SiOAl	2.89	qp	45.22	[335]
	OH	6.75	0.5	44.5	[334]
	2AlOH	7.4	qp	34	[335]
	NaAlSi ₂ O ₆ (jadeite)	O1	3.3	0.9	64
O2		4.1	0.15	59	[110]
O3		5.0	0.5	69	[110]
Mg ₃ Al ₂ Si ₃ O ₁₂ (pyrope)		3.40	0.30	84.0	[110]

Ca ₃ Al ₂ Si ₃ O ₁₂ (grossular)		4.10	0.40	102.0	[110]
1.7Al ₂ O ₃ ·SiO ₂ (mullite)	Oc*	2.0	0.4	40.5	[110]
	Oc	3.3	0.1	76	[110]
	Oab and Od	3.3	0.3	58.5	[110]
Yttrium aluminosilicat glass	br O	3.1	-	54	[336]
	nb O			143	[336]
	nb O			210	[336]
Lanthanum aluminosilicat glass	br O	3.1	-	58	[336]
	nb O			178	[336]
NaAlSi ₃ O ₈ (glass)	SiOSi	5.1	0.15	49	[337]
	SiOSi	5.2	0.2	40	[296]
	SiOAl	3.2	0.05	33	[337]
	SiOAl	3.8	0.2	25	[296]
Na, LiAlSiO ₄ (glasses)	SiOSi	≈4.5-5.0	-	≈49-66	[338]
	SiOAl	≈3.0-3.5	-	≈35-42	[338]
	AlOAl	≈1.7-1.9	-	≈18-22	[338]
14Na ₂ O·4Al ₂ O ₃ ·17B ₂ O ₃ ·65SiO ₂ (glass)	SiOSi	5.1	qp	40	[339]
	SiOB	5.2	qp	57	[339]
	BOB	5.6	qp	62	[339]
	SiOAl	3.6	qp	26	[339]
CaAl ₂ Si ₂ O ₈ (glass)	SiOAl	3.5	-	61	[340]
	nb O	2.9	-	113	[340]
Sodium aluminosilicate glass, NAS, Si/Al=0.7	AlOAl	1.85	qp	19	[273]
Calcium aluminosilicate glass, CAS, Si/Al=0.5	AlOAl	2.4	qp	68	[273]
La, Lu, Sc, Y in aluminosilicate glasses		1.82-3.30	-	140-202	[341]

Other (non-zeolite) phosphorous containing materials

<i>h</i> -P ₂ O ₅	br POP	7.46	0.60	122	[342]
	nb PO	3.96	0.00	80	[342]
KH ₂ PO ₄		5.2	0.55	92	[343]
NH ₄ H ₂ PO ₄		5.1	0.55	93	[343]
α/β-Mg ₂ P ₂ O ₇	nb O	5.27	0.40	82.9	[344]
Na ₄ P ₂ O ₇	2 nb O	3.90/3.90	0.6/0.6	85.7/81.0	[344]
	br O	3.90	0.55	134.3	[344]
Ba ₂ P ₂ O ₇	nb O	4.19	0.26	141.3	[344]
	2 br O	7.25/6.82	0.15/ qp	142.9/134.9	[344]
Sodium phosphate glass	br POP	7.7	0.35	119.1	[345]
51.7Na ₂ O 48.3P ₂ O ₅	nb PONA	4.8	0.15	84.1	[345]
NaPON glass	PONA	4.4	0.2	8.0	[346]
	PON-1/2/3/4	4.3-4.4	0.1-0.3	12.2-15.8	[346]
Sodium borophosphate glass	nb NaOP	4.2	qp	83	[347]
	br POP	7.9	qp	120	[347]
	nb NaOB	4.7	qp	61	[347]
	br BOP	7.1	qp	93	[347]
Ca ₅ (PO ₄) ₃ (OH) (hydroxyapatite)	peak 1/2	4.0/4.1	0.0/0.1	108/115	[343]
CaHPO ₄ ·2H ₂ O	peak 1/2	4.2/4.3	0/0	98/96	[343]
CsH(PO ₃ H)	O1/O4	3.8	0.0	155	[348]
	O2/O5	4.4	0.1	129	[348]
	O3/O6	5.9	0.5	100	[348]

Other (non-zeolite) germanium containing materials

GeO ₂ (quartz)	GeO ₄	7.3	0.48	70	[349, 350]
	O ₄₄	7.05	0.53	49.5	[249]
GeO ₂ (rutile)	OGe ₃	7.5	0.10	160	[349, 350]
	O ₆₆	7.35	0.08	152.2	[249]
GeO ₂ (glass)	GeO ₄	7.1	0.48	70	[350]
	O ₄₄	7.7	qp	42	[249]
Na ₂ Ge ₂ O ₅	nb O	5.95	0.0	38.5	[248]
	O ₄₄	6.05	0.6	61	[248]
Na ₂ GeO ₃	GeO ₄	5.2	0.5	70	[349]
	O ₄₄ O1	5.5	0.70	75	[249]
	nb O	2.5	0.5	47	[349]
	nb O1	5.45	0.00	45.5	[249]
Na ₂ Ge ₄ O ₉	O ₄₄	5.9	0.54	70.0	[249]
	O ₄₆ A	5.9	0.48	117.0	[249]
	O ₄₆ B	5.7	0.48	133.5	[249]
	O ₄₆ C	6.4	0.65	151.0	[249]
Na ₄ Ge ₉ O ₂₀	O ₄₄ /O ₄₆	6.4/5.6	0.65/0.88	70.0/117.0	[249]
	O ₆₆₆	3.75	0.05	133.5	[249]
Na ₂ O·9GeO ₂ (glass)	GeO ₄ & GeO ₆	7.0	0.5	165	[349]
2 9GeO ₂ (glass)	GeO ₄	6.0	0.5	80	[349]
14Na ₂ O·86GeO ₂ (glass)	O ₄₄	7.0	qp	57	[249]
	O ₄₅ /O ₄₆	7.1	qp	97	[249]
	O ₄₅ /O ₄₆	6.3	qp	144	[249]
27Na ₂ O·73GeO ₂ (glass)	nb O	5.9	qp	47	[249]
	O ₄₄	6.6	qp	64	[249]
	O ₄₅ /O ₄₆	6.8	qp	105	[249]
LiTiOGeO ₄	TiOGe	4.8	0.22	148	[301]
HfGeO ₄ (gel)	HfOGe	5.2	0.65	185	[351]
Others					
H ₂ O ₂ (solution) (NQR at 1.5 K)		-	-	180	[352]
		16.31	0.687	-	[353]
NaIO ₄		11.19	0.066	250	[354]
KIO ₄		10.87	0.032	251	[354]
HfO ₂ and hafnates	7 compounds -		-	237.8-331.9	[351]
	nb apical OTi ≈0		-	749	[301]
KReO ₄ (perrhenate)		1.28	0.25	137	[355]
NH ₄ ReO ₄ (perrhenate)		1.25	0.16	133	[355]
TiO ₂ (rutile)	TiOTi	1.5	0.87	596.5	[356]
	TiOTi	< 1.5	-	590	[267]
(anatase)	TiOTi	< 1.1	-	558	[267]
Ti ₂ O ₃ (corundum)	TiOTi	< 2.6	-	503	[267]
K(Mg _{2.5} Al _{0.5})[Al _{1.5} Si _{2.5} O ₁₀](OH)F (phlogopite)					
	H-O- ^[6] (Mg,Al)	5.5	0.6	78.6	[357]
	Si-O- ^[6] (Mg,Al)	1.5	0.7	71.1	[357]
	Si-O-Si 1	2.8	0.3	46.9	[357]
	Si-O- ^[4] Al	2.2	0.7	42.5	[357]
	Si-O-Si 2	2.7	0.3	33.8	[357]
	Al-O-Al	2.4	0.7	25.0	[357]
Li ₂ O ₂	LiOLi	18.0	0.00	227	[358]
Li ₂ , Ca, Sr, BaTiO ₃	5 compounds -		-	372-564	[275]
Li ₂ , Na ₂ , Ca, Sr, BaZrO ₃	5 compounds -		-	280-376	[275]

Li ₂ , SrSnO ₃	3 compounds -	-	-	85-423	[275]	
LiNbO ₃		3.4 (maximum)-	-	504	[275]	
SiO ₂ /TiO ₂ (gel)	SiOSi	5.1	0.0	42	[359]	
QTiAc: TEOS, Ti(OPr ⁱ) ₄ , AcacH	SiOTi	2.7	0.0	174	[359]	
	SiOTi	3.0	0.0	314	[359]	
	nb OTi ₄ / nb OTi ₃	-	-	375/542	[359]	
	tetragonal	< 1.4	-	383	[267]	
ZrO ₂	tetragonal	0.26	0.68	384	[360]	
(baddeleyite)	2 monoclinic	< 0.9/< 1.0	-	325/402	[267]	
ZnO nanoparticle	HOZn ₃	5.6	-	-4.5	[268]	
	OZn ₃	4.8	-	-6.1	[268]	
	OZn ₄	1.5	-	-3.3	[268]	
	OZn ₄	<0.5	-	from -14 to -38	[268]	
ZnO (wurtzite)		< 1.4	-	383	[267]	
SnO (litharge)		< 2.3	-	251	[267]	
La ₂ O ₃	hexagonal	< 1.4/2.2	-	469/590	[267]	
HfO ₂ (baddeleyite)		< 1.1	-	267/335	[267]	
PbO (litharge)		< 0.9	-	294	[267]	
M _x O _y -PDMS-hybrides	SiOTa	3.0	-	243	[361]	
	nb OTa ₂	-	-	440	[361]	
	SiONb	-	-	275	[361]	
	nb ONb ₂	-	-	545	[361]	
	SiOTi	3.0	-	332	[361]	
	nb OTi ₂	-	-	719	[361]	
	SiOZr	3.4	-	219	[361]	
	nb OZr ₃	-	-	402	[361]	
	V ₂ O ₅ (crystalline)	O _{1A}	0.9	0.6	1213	[362]
O _{1B}		4.0	0.7	400	[362]	
O _{1C}		3.3	0.6	0	[362]	
Na ₂ Al ₂ B ₂ O	O1/ O2	3.7/1.4	0.77/0	65.0/24.5	[134]	
SrB ₄ O ₇	BO	5.50/5.60/5.55	0.25-0.65	79.8/78.2/72.1	[363]	
	Tricluster	6.6	0.2	68.0	[363]	
Sodium aluminoborate glass NAB-40-20-40	AlOAl	1.7	qp	18.6	[364]	
	AlOB	3.7	qp	44.1	[364]	
	AlOB	4.1	qp	62.7	[364]	
	B nb O	4.0	qp	83	[364]	
	BOB	4.8/5.0	qp	8/995	[364]	
	NAB-30-5-65	AlOB	4.3	qp	61.9	[364]
		B nb O	4.0	qp	83	[364]
		2 BOB	4.8/5.4	qp/ qp	87.1/96	[364]
	Borate, borosilicate, boroaluminate glasses	SiOSi	5.4 and 4.9	qp	37 and 51	[365]
BOB		5.5 and 5.1	qp	92 and 82	[365]	
SiOB		5.6	qp	64	[365]	
Si[B]ONa		2.2	qp	35	[365]	
Si[B]OK		2.1	qp	76	[365]	
AlOB		4.1	qp	59	[365]	
Al[B]ONa		1.7	qp	16	[365]	
Titania based hybrids	POTi 4	5.2	0.15	152.5	[366]	
	POTi 1-2-3	5.3	0.15	215.0	[366]	
Mg(OH) ₂ (brucite)	MgOH	6.8	0	20	[367]	
	MgOH	6.8	0.0	25	[286]	
Mg(OH) ₂	MgOH	6.8	0.0	25	[266]	
Ba(ClO ₃) ₂ ·H ₂ O	H ₂ O	6.8	1.00	22	[343]	

Ba ₂ In ₂ O ₅ (brownmillerite)	site A (O1/O3)	5.0	0.2	189	[368]
	site B (O2)	5.8	0.2	146	[368]
Ba ₂ In ₂ O ₄ (OH) ₂	site A/ site B	4.5/4.1	0.0/0.7	188/173	[369]
	site C/ site D	4.2/4.8	0.5/0.7	152/97	[369]
LaSiO ₂ N (La-N-wollastonite)	nb OSi	2.4	-	215	[370]
La ₄ Si ₂ O ₇ N ₂	ionic	≈0	-	575	[370]
	nb OSi	2.4	-	220	[370]
La ₄ SiAlO ₈ N	ionic	≈0	-	570	[370]
	nb OAl	1.8	-	311	[370]
	nb OSi	3.1	-	246	[370]
La ₁₀ Si ₆ O ₂₄ N ₂	ionic	<1	-	596	[370]
NaNO ₂		11.05	0.58	643	[371]
Na ₂ (ONNO ₂)		13.5	0.40	265	[372]
[HONH ₃]Cl		14.7	0.71	90	[372]
LiOH (NQR)		-7.283	0.07	-	[373]
NaOH (NQR at 77 K))		-7.590	0.07	-	[373]
KOH (NQR at 77 K))		-7.140	0.08	-	[373]
β-Ba(OH) ₂ (NQR at 77 K))		-7.124	0.07	-	[373]
Sr(OH) ₂ (NQR at 77 K))		-7.267	0.08	-	[373]
Ca(OH) ₂		6.5	0.00	62	[343]
CaOH		6.5	0.3	71	[282]
CaCO ₃		6.97	1	204	[374]
ThO ₂		very small		576	[375]
UO ₂		very small		717	[375]
NpO ₂		very small		475	[375]
PuO ₂		very small		54	[375]
AmO ₂		very small		-754	[375]
Y ₂ Sn ₂ O ₇	O1	≈0.02	0.14	384.0	[376]
	O2	3.2	0.36	172.5	[376]
Y ₂ Ti ₂ O ₇	O1	≈0.02	0.13	386.1	[376]
	O2	0.7	0.50	454.6	[376]
La ₂ Sn ₂ O ₇	O1	≈0.02	0.20	641.5	[376]
	O2	3.3	0.90	222.0	[376]
Y ₂ Sn ₂ O ₇	O1	0.02	-	384.0	[377]
Y ₂ Sn ₂ O ₇	O2	3.2	0.4	172.5	[377]
Y ₂ Ti ₂ O ₇	O1	0.02	-	386.1	[377]
Y ₂ Ti ₂ O ₇	O2	0.7	0.5	454.6	[377]
La ₂ Sn ₂ O ₇	O1	0.02	-	641.5	[377]
La ₂ Sn ₂ O ₇	O2	3.3	0.9	220.0	[377]
La ₂ Zr ₂ O ₇	O1	0.02	-	626.3	[377]
La ₂ Zr ₂ O ₇	O2	1.5	0.4	394.0	[377]
La ₂ Hf ₂ O ₇	O1	0.02	-	629.9	[377]
La ₂ Hf ₂ O ₇	O2	1.4	0.6	350.8	[377]
La ₂ Mg ₃ (NO ₃) ₁₂ ·24H ₂ ¹⁷ O (LMN)	H ₂ O-1	7.1	0.8	-5	[378]
	H ₂ O-2	7.1	0.8	-2	[378]
	H ₂ O-3	6.6	0.8	0	[378]
	H ₂ O-4	6.8	0.9	3	[378]
α-TeO ₂		7.39	0.42	179	[379]
La ₂ NiO _{4+δ}	8 sites	<4.6/≈4.6	-	532 and 3640-5590	[380]
Ba(ClO ₃) ₂ ·H ₂ O	H ₂ O	6.91	0.97	19.7	[381]
Li ₂ SO ₄ ·H ₂ O	H ₂ O	6.6	0.86	-7.1	[381]
K ₂ C ₂ O ₄ ·H ₂ O	H ₂ O	6.62	0.95	1.1	[381]
NaClO ₄ ·H ₂ O	H ₂ O	7.35	0.72	-17	[381]

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