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Subvolume I 2

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## Preface

The Landolt-Börnstein Volume 27 deals with the magnetic properties of non-metallic inorganic compounds based on transition elements, such as there are pnictides, chalcogenides, oxides, halides, borates, and finally phosphates and silicates, the latter presented in this subvolume I. A preliminary survey of the contents of all subvolumes that have already appeared or have been planned to appear is printed on the inside of the front cover.

The silicates are very complex systems, intensively studied in literature. These cover large classes of minerals as well as synthetic samples. In analyzing their magnetic and magnetically related properties we followed the classification given by the Mineral Reference Manual (E.H. Nickel, N.C. Nickols, Van Nostrand Reinhold, 1991). Individual chapters are dedicated to orthosilicates, sorosilicates, cyclosilicates, inosilicate, phyllosilicates and tectosilicates. Due to the huge amount of data these chapters had to be spread over several subvolumes I1, I2, etc.. - In each chapter the different groups of minerals and synthetic silicates were distinctly analyzed in various sections. For each group, additional silicate minerals, more recently reported, as well as synthetic samples having related compositions and/or crystal structures were also considered. The silicates included in each section were firstly tabulated, mentioning their compositions. The solid solutions between the end member compounds were also described. The space groups and lattice parameters for most silicates were tabulated. Crystal structures of representative silicates were discussed in more detail and the atomic positions were given. In addition to magnetic properties, the results of neutron diffraction studies, nuclear gamma resonance, nuclear magnetic resonance, transport properties, dielectric and optical data were reviewed. Short comments of the properties given by various authors were made, when the data reported by various authors were different. Then, representative results were given in tables and figures. For many systems, only crystal structures are known. Thus, further opportunities appear for analyses of their physical properties.

The present volume I2 contains two indexes of substances covered herein: A) an alphabetical index of element systems (listing the systems of alphabetically ordered elements of the substances and their chemical formulae) and B) an alphabetical index of mineral names.

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Aachen, August 2004

**The Editor**

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## List of frequently used symbols and abbreviations

## Symbols

Symbol	Unit	Property
$a, b, c$	Å	lattice parameters
$a^*, b^*, c^*$	Å <sup>-1</sup>	lattice parameters in reciprocal space
$A$	cm <sup>-1</sup>	hyperfine constant, exchange parameter
$A$	%	relative area of NGR spectrum
$B$	T	magnetic induction
$B_{\text{hf}}$		hyperfine magnetic field
$B, B_{\text{eq}}, B_{\text{iso}}$	Å <sup>2</sup>	isotropic temperature parameter
$c_{ij}$	Pa	elastic stiffnesses
$C$	emu K f.u. <sup>-1</sup> = cm <sup>3</sup> K f.u. <sup>-1</sup>	Curie constant per formula unit
$C$	J g <sup>-1</sup> K <sup>-1</sup> , J mol <sup>-1</sup> K <sup>-1</sup>	heat capacity
$C_p$		heat capacity at constant pressure
$C_v$		heat capacity at constant volume
$C_{\text{magn}}$		magnetic heat capacity
$d$	Å	thickness
$d_{ij}$	C N <sup>-1</sup>	piezoelectric constant
$D$	cm <sup>-1</sup>	Hamiltonian parameter
$Dq$	cm <sup>-1</sup>	crystal field splitting parameter
$DH$	mm s <sup>-1</sup> , Hz	linewidth of NGR or NMR line
$e$	C	electron charge
$e_{ij}$		strain tensor
$E$	Pa	Young modulus
$E$	V cm <sup>-1</sup>	electric field strength
$E$	cm <sup>-1</sup>	Hamiltonian parameter
$E$	eV	energy
$E_a$		activation energy (for conductivity,...)
$f$	Hz	frequency
$g$		spectroscopic splitting factor
$G$	Pa	torsional (shear) modulus
$h$		Planck constant
$\mathbf{H}$		Hamiltonian
$\Delta H$	eV	enthalpy
$H$	Oe, A m <sup>-1</sup>	magnetic field (strength), sometimes given as $\mu_0 H$ in tesla (T))
$I$		nuclear spin quantum number
$I$	various units	intensity
$J$	eV	exchange interaction energy ( $J/k_B$ in K)
$J_{x,y}, J_3$		exchange interaction energies (for special meaning see corresponding text, tables or figures)
$k$	Å <sup>-1</sup>	wavevector
$k_B$	J K <sup>-1</sup>	Boltzmann constant
$K, K_T$	Pa	bulk modulus ( $K'$ : first pressure derivative of bulk modulus)
$l$	m	length
$M$	G	magnetization

Symbol	Unit	Property
$n$		refractive index
$\Delta n$		birefringence
$p$	Pa, bar	hydrostatic pressure
$p$	$\mu_B$	magnetic moment (sometimes also $M$ is used)
$p_A$		magnetic moment per atom
$p_{\text{eff}}$		effective (paramagnetic) moment
$p_M$		magnetic moment per ion M
$p_o$		ordered magnetic moment
$p_s$		spontaneous magnetic moment
$p_3$	$\text{C K}^{-1} \text{ m}^2$	pyroelectric coefficient
$q$	$\text{\AA}^{-1}$	wavevector (also dimensionless wavevector component)
$\Delta Q$	$\text{mm s}^{-1}$	quadrupole splitting
$Q$		order parameter
$r$	$\text{\AA}$	radius, distance
$r_{M,(R)}$		radius of ion M (R)
$R$		reflectivity
$S$	$\mu\text{V K}^{-1}$	Seebeck coefficient (thermoelectric power)
$S$		spin quantum number
$S$	$\text{J K}^{-1} \text{ mol}^{-1}$	entropy
$T$		transmission
$T$	K, $^{\circ}\text{C}$	temperature
$T_{\text{IC-N}}$		transition temperature IC to N phase
$T_{\text{LI}}$		lock-in phase transition temperature
$T_{\text{ord}}$		ordering temperature
$T_N$		Néel temperature
$T_t$		(crystallographic) transition temperature
$U_{\text{eq}}$	$\text{\AA}^2$	temperature parameter
$v$	$\text{mm s}^{-1}$ , $\text{m s}^{-1}$	velocity (mostly of absorber in Mössbauer effect)
$V$	$\text{\AA}^3$	(unit cell) volume
$V^0$	deg	angle between optical axes
$V_{zz}$	$\text{V cm}^{-2}$	main component of the electric field gradient tensor
$x, y, z$		fractional coordinates of atoms in the unit cell
$X, Y, Z$		principal directions
$\alpha$	$\text{cm}^{-1}$	absorption (extinction) coefficient
$\alpha$	$\text{K}^{-1}$	linear thermal expansion coefficient
$\alpha, \beta, \gamma$	deg	(unit cell) angles
$\beta$	$\text{bar}^{-1}$ , $\text{Pa}^{-1}$	linear compressibility
$\beta_{ij}$		anisotropic temperature parameter
$\Gamma$	$\text{mm s}^{-1}$	linewidth of NGR line
$\Delta_{\text{corr}}$	$\text{cm}^{-1}$	effective linewidth of peaks in IR spectra
$\delta$	ppm, $\text{mm s}^{-1}$	chemical shift, isomer shift
$\varepsilon = \varepsilon_1 - i \varepsilon_2$		dielectric constant
$\varepsilon_1, \varepsilon_2$		real, imaginary part of dielectric constant
$\varepsilon_i$		spontaneous strain
$\eta$		asymmetry parameter, order parameter
$\theta$	deg	angle (bond angle, ...)
$\Theta$	K	paramagnetic Curie temperature
$\lambda$	nm, $\mu\text{m}$ , $\text{\AA}$	wavelength



Symbol	Unit	Property
$\lambda$	$\text{s}^{-1}$	relaxation rate (in NGR)
$\mu_{\text{B}}$	$\text{J T}^{-1}$	Bohr magneton
$\nu$		Poisson ratio
$\nu$	$\text{Hz}$	frequency
$\nu_{\text{as}}$	$\text{Hz}$	"antisymmetric" frequency
$\nu_{\text{s}}$	$\text{Hz}$	"symmetric" frequency
$\nu_{\text{OH}}$	$\text{Hz}$	frequency of O-H stretching vibration
$\nu_{\text{L}}$	$\text{Hz}$	Larmor frequency
$\bar{\nu}$	$\text{cm}^{-1}$	wavenumber
$\Delta\bar{\nu}$	$\text{cm}^{-1}$	Raman shift
$\rho$	$\text{kg m}^{-3}$	density
$\rho$	$\Omega \text{ m}$	resistivity
$\sigma$	$\Omega^{-1} \text{ m}^{-1}, \Omega^{-1} \text{ cm}^{-1}$	electrical conductivity
$\sigma$	$\text{emu g}^{-1} = \text{G cm}^3 \text{ g}^{-1},$ $\text{A m}^2 \text{ kg}^{-1}$	magnetic moment per unit mass = specific magnetization
$\sigma_{\text{s}}$		spontaneous magnetization
$\xi$		order parameter
$\tau$	$\text{s}$	relaxation time
$\chi_{\text{A}}$	$\mu_{\text{B}} \text{T}^{-1} \text{ atom}^{-1}$	magnetic susceptibility per atom
$\chi_{\text{g}}$	$\text{emu g}^{-1} = \text{cm}^3 \text{ g}^{-1},$ $\text{m}^3 \text{ kg}^{-1}$	magnetic susceptibility per gram
$\chi_{\text{m}}$	$\text{emu mol}^{-1} = \text{cm}^3 \text{ mol}^{-1},$ $\text{m}^3 \text{ mol}^{-1}$	magnetic susceptibility per mole
$\omega$	$\text{s}^{-1}$	angular frequency
$\omega_{\text{Q}}$		quadrupole frequency

### Abbreviations

ac	alternating current
apfu	atom per formula unit
AF	antiferromagnetic
c, cr	mostly as subscript: critical
calc	calculated
CFSE <sup>(ex)</sup>	(excess) crystal field stabilization energy
CN	coordination number
dc	direct current
1D, 2D, 3D	one-, two-, three-dimensional
DAS	dynamical angle spinning
eff	mostly as subscript: effective
emu	electromagnetic unit
exp	experimental
ED	electron diffraction
EFG	electric field gradient
EPR	electron paramagnetic resonance
EXAFS	extended X-ray absorption fine structure
FTIR	Fourier transform infrared spectroscopy
FU, f.u.	formula unit
HAF	Heisenberg antiferromagnetic (system)
HRTEM	high resolution transmission electron microscopy

---

HT	high temperature $T > 300$ K
IC	incommensurate (phase)
IR	infrared
IVCT	intervalence charge transfer
LMCT	ligand-metal charge transfer
LRO	long range order
LT	low temperature
magn	mostly as subscript: magnetic
max	mostly as subscript: maximum
min	mostly as subscript: minimum
M	metal
MAS	magic angle spinning
MF	mean field
MP	mixed powder
$\mu$ SR	muon spin relaxation
N	normal (phase, structure)
NGR	nuclear gamma resonance (Mössbauer effect)
NMR	nuclear magnetic resonance
NN	nearest neighbor
pfu	per formula unit
PAC	perturbed angular correlation
R	rare earth element
RPA	random phase approximation
RT	room temperature
SG	sol-gel
SHG	second-harmonic generation
T	mostly transition element
TED	transmission electron diffraction
TEM	transmission electron microscopy
XANES	X-ray absorption near edge spectroscopy
$\perp, \parallel$	perpendicular, parallel to a crystallographic axis
$\square$	vacancy

---

## Definitions, units and conversion factors

In the SI, units are given for both defining relations of the magnetization,  $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$  and  $\mathbf{B} = \mu_0\mathbf{H} + \mathbf{M}$ , respectively.  $\mu_0 = 4\pi \cdot 10^{-7} \text{ Vs A}^{-1} \text{ m}^{-1}$ ,  $A$ : molar mass,  $\rho$ : mass density,  $\mathbf{P}$ : magnetic moment,  $\mathbf{M}$ : magnetic moment per unit volume (magnetization, magnetic polarization).

Quantity	cgs/emu	SI	
$\mathbf{B}$	$\text{G} = (\text{erg cm}^{-3})^{1/2}$ $1 \text{ G} \hat{=}$	$\text{T} = \text{Vs m}^{-2}$ $10^{-4} \text{ T}$	
$\mathbf{H}$	$1 \text{ Oe} = (\text{erg cm}^{-3})^{1/2}$ $1 \text{ Oe} \hat{=}$	$\text{A m}^{-1}$ $10^3/4\pi \text{ A m}^{-1}$	
$\mathbf{M}$	$\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}$ $\text{G}$ $1 \text{ G} \hat{=}$	$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$ $\text{A m}^{-1}$ $10^3 \text{ A m}^{-1}$	$\mathbf{B} = \mu_0 \mathbf{H} + \mathbf{M}$ $\text{T}$ $4\pi \cdot 10^{-4} \text{ T}$
$\mathbf{P}$	$\mathbf{P} = \mathbf{MV}$ $\text{G cm}^3$ $1 \text{ G cm}^3 \hat{=}$	$\mathbf{P} = \mathbf{MV}$ $\text{A m}^2$ $10^{-3} \text{ A m}^2$	$\mathbf{P} = \mathbf{MV}$ $\text{V s m}$ $4\pi \cdot 10^{-10} \text{ V s m}$
$\sigma$	$\sigma = \mathbf{M}/\rho$ $\text{G cm}^3 \text{ g}^{-1}$ $1 \text{ G cm}^3 \text{ g}^{-1} \hat{=}$	$\sigma = \mathbf{M}/\rho$ $\text{A m}^2 \text{ kg}^{-1}$ $1 \text{ A m}^2 \text{ kg}^{-1}$	$\sigma = \mathbf{M}/\rho$ $\text{V s m kg}^{-1}$ $4\pi \cdot 10^{-7} \text{ V s m kg}^{-1}$
$\sigma_m$	$\sigma_m = \sigma A$ $\text{G cm}^3 \text{ mol}^{-1}$ $1 \text{ G cm}^3 \text{ mol}^{-1} \hat{=}$	$\sigma_m = \sigma A$ $\text{A m}^2 \text{ mol}^{-1}$ $10^{-3} \text{ A m}^2 \text{ mol}^{-1}$	$\sigma_m = \sigma A$ $\text{V s m mol}^{-1}$ $4\pi \cdot 10^{-10} \text{ V s m mol}^{-1}$
$\chi$	$\mathbf{P} = \chi\mathbf{H}$ $\text{cm}^3$ $1 \text{ cm}^3 \hat{=}$	$\mathbf{P} = \chi\mathbf{H}$ $\text{m}^3$ $4\pi \cdot 10^{-6} \text{ m}^3$	$\mathbf{P} = \chi\mu_0\mathbf{H}$ $\text{m}^3$ $4\pi \cdot 10^{-6} \text{ m}^3$
$\chi_v$	$\chi_v = \chi/V$ $\text{cm}^3 \text{ cm}^{-3}$ $1 \text{ cm}^3 \text{ cm}^{-3} \hat{=}$	$\chi_v = \chi/V$ $\text{m}^3 \text{ m}^{-3}$ $4\pi \text{ m}^3 \text{ m}^{-3}$	$\chi_v = \chi/V$ $\text{m}^3 \text{ m}^{-3}$ $4\pi \text{ m}^3 \text{ m}^{-3}$
$\chi_g$	$\chi_g = \chi_v/\rho$ $\text{cm}^3 \text{ g}^{-1}$ $1 \text{ cm}^3 \text{ g}^{-1} \hat{=}$	$\chi_g = \chi_v/\rho$ $\text{m}^3 \text{ kg}^{-1}$ $4\pi \cdot 10^{-3} \text{ m}^3 \text{ kg}^{-1}$	$\chi_g = \chi_v/\rho$ $\text{m}^3 \text{ kg}^{-1}$ $4\pi \cdot 10^{-3} \text{ m}^3 \text{ kg}^{-1}$
$\chi_m$	$\chi_m = \chi_g A$ $\text{cm}^3 \text{ mol}^{-1}$ $1 \text{ cm}^3 \text{ mol}^{-1} \hat{=}$	$\chi_m = \chi_g A$ $\text{m}^3 \text{ mol}^{-1}$ $4\pi \cdot 10^{-6} \text{ m}^3 \text{ mol}^{-1}$	$\chi_m = \chi_g A$ $\text{m}^3 \text{ mol}^{-1}$ $4\pi \cdot 10^{-6} \text{ m}^3 \text{ mol}^{-1}$

### Experimental errors

In this volume, experimental errors are given in parentheses referring to the last decimal places. For example, 1.352(12) stands for  $1.352 \pm 0.012$ , and 342.5(21) stands for  $342.5 \pm 2.1$ .