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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. They 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 I4 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, March 2006

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 ⁻¹	lattice parameters in reciprocal space
A	cm ⁻¹	hyperfine constant
A	%	relative area of NGR spectrum
B	T	magnetic induction
B_{eff}		effective magnetic field
B_{hf}		hyperfine magnetic field
B	cm ⁻¹	Racah parameter
B, B_{eq}	Å ²	isotropic temperature parameter
c_{ij}	Pa, bar, N m ⁻²	elastic stiffnesses
C	emu K g ⁻¹ = cm ³ K g ⁻¹ ;	Curie constant per unit mass
	emu K mol ⁻¹ = cm ³ K mol ⁻¹	Curie constant per mole
C	J g ⁻¹ K ⁻¹ , J mol ⁻¹ K ⁻¹	heat capacity
C_p		heat capacity at constant pressure
C_{magn}		magnetic heat capacity
d	Å	distance, diameter
D	cm ⁻¹	Hamiltonian parameter
DH	mm s ⁻¹	linewidth of NGR or NMR line
Dq	cm ⁻¹	crystal field splitting parameter
e	C	electron charge
e^2qQ/h	Hz	nuclear quadrupole coupling constant
E	V cm ⁻¹	electric field strength
E	cm ⁻¹	Hamiltonian parameter
E	eV	energy
E_a		activation energy
E_r		relative energy
f	Hz	frequency
f_{O_2}	atm, bar	oxygen fugacity
g		spectroscopic splitting factor
G	Pa	torsional (shear) modulus
h		Planck constant
\mathbf{H}		Hamiltonian
ΔH	J mol ⁻¹	enthalpy
H	Oe, A m ⁻¹	magnetic field (strength), mostly given as $\mu_0 H$ in tesla (T))
H_c		critical field, coercive field
H_s		spin flop transition field
I	various units	intensity
J, j	eV	exchange interaction energy (J/k_B in K)
$J, J', J_{1,2}$		exchange interaction energies (for special meaning see corresponding text, tables or figures)
k	Å ⁻¹	wavevector
k_B	J K ⁻¹	Boltzmann constant

Symbol	Unit	Property
K	erg cm^{-3}	anisotropy constant
$K_{(0)}$	Pa	(zero-pressure or isothermal) bulk modulus (K' : first pressure derivative of bulk modulus)
K_D		equilibrium distribution coefficient
L		orbital angular momentum quantum number
M	G	magnetization
n		refractive index
p	Pa, bar, atm	hydrostatic pressure
p_{O_2}		oxygen partial pressure
p	μ_B	magnetic moment
p_{eff}		effective (paramagnetic) moment
p_M		magnetic moment per ion M
$P(B_{\text{hf}})$		hyperfine distribution (probability)
ΔQ	mm s^{-1}	quadrupole splitting
Q, Q_D, Q_{OD}		order parameter
r, R	\AA	(ionic) radius, distance
R	$\text{J K}^{-1} \text{mol}^{-1}$	gas constant
R		reflectivity
S	$\text{J K}^{-1} \text{mol}^{-1}$	entropy
S_{magn}		magnetic part of entropy
S		spin quantum number
S	$\mu\text{V K}^{-1}$	Seebeck coefficient (thermoelectric power)
t		stacking vector
t	μm	thickness
t	s, min, h	time (delay time, annealing time, ...)
T	K, $^{\circ}\text{C}$	temperature
T_0, T_c		(mostly) phase transition temperature
T_C		Curie temperature
T_g		glass transition temperature
T_m, T_M, T_{max}		maximum temperature (of e.g. χ vs T plot); T_m also ordering temperature
T_N		Néel temperature
T_{SC}		spin-Peierls transition temperature
T_{SP}		spin-canting temperature
T_1	s	spin lattice relaxation time
v	mm s^{-1}	velocity (of absorber in Mössbauer effect)
V	\AA^3	(unit cell) volume
ν^0	deg	angle between optical axes
V_{zz}	V cm^{-2}	main component of the electric field gradient tensor
$X_{(\text{Fe})}$		occupancy of sites (by Fe atoms)
x, y, z		fractional coordinates of atoms in the unit cell
X, Y, Z		principal directions
α	K^{-1}	linear thermal expansion coefficient
α	cm^{-1}	absorption coefficient
α, β, γ	deg	(unit cell) angles
β	$\text{bar}^{-1}, \text{Pa}^{-1}$	linear compressibility
Δ	$\text{eV}, \text{cm}^{-1}$	spin gap, also for crystal field splitting energy
δ	ppm, mm s^{-1}	chemical shift, isomer shift
δ_i		intrinsic isomer shift
δ_{SOD}		second order Doppler shift

Symbol	Unit	Property
$\varepsilon = \varepsilon_1 - i \varepsilon_2$		dielectric constant
$\varepsilon_1, \varepsilon_2$		real, imaginary part of dielectric constant
η		asymmetry parameter
θ	deg	angle (scattering angle, ...)
Θ	K	paramagnetic Curie temperature
Θ_D	K	Debye temperature
Θ_M	K	lattice temperature
λ	nm, μm	wavelength
μ_B	J T^{-1}	Bohr magneton
ν	Hz	frequency, also used for wavenumber
$h\nu$	eV, Ry	photon energy
$\bar{\nu}$	cm^{-1}	wavenumber
$\Delta\bar{\nu}$	cm^{-1}	Raman shift
ξ	cm^{-1}	spin orbit coupling
ρ	$\Omega \text{ m}$	resistivity
ρ	$e \text{ \AA}^{-3}$	electron density (distribution)
σ	$\Omega^{-1} \text{ cm}^{-1}$	electrical conductivity
σ	$\text{emu g}^{-1} = \text{G cm}^3 \text{ g}^{-1}$	magnetic moment per unit mass = specific magnetization
τ	s	relaxation time, contact time
φ, ϕ	deg	angle (for special definition see text, tables or figures)
χ	$\text{emu}, \mu_B \text{T}^{-1} \text{ atom}^{-1},$ $\text{J T}^{-2} \text{ kg}^{-1}$	magnetic susceptibility
χ_g	$\text{emu g}^{-1} = \text{cm}^3 \text{ g}^{-1},$ $\text{m}^3 \text{ kg}^{-1}$	magnetic susceptibility per gram
χ_m	$\text{emu mol}^{-1} = \text{cm}^3 \text{ mol}^{-1},$ $\text{m}^3 \text{ mol}^{-1}$	magnetic susceptibility per mole
ω	s^{-1}	angular frequency
ω_L		Larmor frequency

Abbreviations

ac	alternating current
apfu	atom per formula unit
Ae	aegirine
AF	antiferromagnetic
ASM	astrophyllite group of minerals
br	(subscript) bridging (atoms)
c, cr	mostly as subscript: critical
calc	calculated
CAF	chain-arrangement fault
CaTs	calcium Tschermak's pyroxene
CFs	clinoferrosilite
CFSE	crystal field stabilization energy
CJT	clinojinthompsonite
CMF	chain-multiplicity faults
CP	cross polarization (spectrum)
CPM	chain periodicity fault
CPx	clinopyroxene

CSH	calcium silicate hydrate
CT	charge transfer
dc	direct current
1D, 2D, 3D	one-, two-, three-dimensional
Di	diopside
DSC	differential scanning calorimeter (analysis)
eff	mostly as subscript: effective
emu	electromagnetic unit
exp	experimental
EFG	electric field gradient
En	enstatite
EPR	electron paramagnetic resonance
EXAFS	extended X-ray absorption fine structure
FC	field cooled
Fs	ferrosilite
FTIR	Fourier transform infrared spectroscopy
FU, f.u.	formula unit
Hd	hedenbergite
HP	high pressure
HPCEn	high-pressure clinoenstatite
HPCFs	high-pressure clinoferrosilite
HPCPx	high-pressure clinopyroxene
HRTEM	high-resolution transmission electron microscopy
HT	high temperature
HTCEn	high-temperature clinoenstatite
HTCFs	high-temperature clinoferrosilite
HTCPx	high-temperature clinopyroxene
HTOEn	high-temperature orthoenstatite
IR	infrared
IVCT	intervalence charge transfer
Jd	jadeite
Jo	johannsenite
JT	jimthompsonite
Kan	kanoite
Ko	kosmochlor
LCEn	low clinoenstatite
LCFs	low clinoferrosilite
LCPx	low clinopyroxene
LRO	long-range order
LTOEn	low-temperature orthoenstatite
magn	mostly as subscript: magnetic
max	mostly as subscript: maximum
min	mostly as subscript: minimum
M	metal
MAS	magic angle spinning
MD	molecular dynamics (simulation)
MDO	maximum degree of disorder
(M)HFD	(magnetic) hyperfine field distribution
MIR	mid-infrared
ND	neutron diffraction
NGR	nuclear gamma resonance (Mössbauer effect)
NIR	near infrared
NMR	nuclear magnetic resonance

NN	nearest neighbor
NNN	next nearest neighbor
o	octahedrally coordinated cations
obs	observed
O _{br}	bridging oxygen
O/D	order/disorder (process)
OEn	orthoenstatite
OFs	orthoferrosilite
O _{nbr}	nonbridging oxygen
OPx	orthopyroxene
ORTEP	Oak Ridge Thermal Ellipsoid Plot Program
p	powder
pc	polycrystal
pfu	per formula unit
PEn	protoenstatite
PG	pargasite
PIB	potential induced breathing (model)
PPx	protopyroxene
PWo	pseudowollastonite
Pxm	Pyroxmangite
QSD	quadrupole splitting distribution
R	rare earth element
RD	random distribution (model)
Rhd	rhodonite
RT	room temperature
SAED	selected area electron diffraction
sc, s.c.	single crystal
SRO	short-range order
SSMEG	shell stabilized modified electron gas (model)
T	(sites of) tetrahedron, tetrahedral, mostly: tetrahedrally coordinated cations
TCS	triple-chain silicate
TEM	transmission electron microscopy
TR, Tr	tremolite
Wo	wollastonite
XANES	X-ray absorption near edge spectroscopy
XAS	X-ray absorption spectroscopy
XRD	X-ray diffraction
ZFC	zero-field cooled
⊥,	perpendicular, parallel to a crystallographic axis
□	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, ρ : mass density, \mathbf{P} : magnetic moment, \mathbf{M} : magnetic moment per unit volume (magnetization, magnetic polarization).

Quantity	cgs/emu	SI	
\mathbf{B}	$G = (\text{erg cm}^{-3})^{1/2}$ $1 G \hat{=}$	$T = \text{Vs m}^{-2}$ $10^{-4} T$	
\mathbf{H}	$1 \text{ Oe} = (\text{erg cm}^{-3})^{1/2}$ $1 \text{ Oe} \hat{=}$	A m^{-1} $10^3/4\pi \text{ A m}^{-1}$	
\mathbf{M}	$\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}$ G $1 G \hat{=}$	$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$ A m^{-1} 10^3 A m^{-1}	$\mathbf{B} = \mu_0 \mathbf{H} + \mathbf{M}$ T $4\pi \cdot 10^{-4} T$
\mathbf{P}	$\mathbf{P} = \mathbf{MV}$ $G \text{ cm}^3$ $1 G \text{ cm}^3 \hat{=}$	$\mathbf{P} = \mathbf{MV}$ A m^2 10^{-3} A m^2	$\mathbf{P} = \mathbf{MV}$ V s m $4\pi \cdot 10^{-10} \text{ V s m}$
σ	$\sigma = \mathbf{M}/\rho$ $G \text{ cm}^3 \text{ g}^{-1}$ $1 G \text{ cm}^3 \text{ g}^{-1} \hat{=}$	$\sigma = \mathbf{M}/\rho$ $\text{A m}^2 \text{ kg}^{-1}$ $1 \text{ A m}^2 \text{ kg}^{-1}$	$\sigma = \mathbf{M}/\rho$ V s m kg^{-1} $4\pi \cdot 10^{-7} \text{ V s m kg}^{-1}$
σ_m	$\sigma_m = \sigma A$ $G \text{ cm}^3 \text{ mol}^{-1}$ $1 G \text{ cm}^3 \text{ mol}^{-1} \hat{=}$	$\sigma_m = \sigma A$ $\text{A m}^2 \text{ mol}^{-1}$ $10^{-3} \text{ A m}^2 \text{ mol}^{-1}$	$\sigma_m = \sigma A$ V s m mol^{-1} $4\pi \cdot 10^{-10} \text{ V s m mol}^{-1}$
χ	$\mathbf{P} = \chi \mathbf{H}$ cm^3 $1 \text{ cm}^3 \hat{=}$	$\mathbf{P} = \chi \mathbf{H}$ m^3 $4\pi \cdot 10^{-6} \text{ m}^3$	$\mathbf{P} = \chi \mu_0 \mathbf{H}$ m^3 $4\pi \cdot 10^{-6} \text{ m}^3$
χ_v	$\chi_v = \chi/V$ $\text{cm}^3 \text{ cm}^{-3}$ $1 \text{ cm}^3 \text{ cm}^{-3} \hat{=}$	$\chi_v = \chi/V$ $\text{m}^3 \text{ m}^{-3}$ $4\pi \text{ m}^3 \text{ m}^{-3}$	$\chi_v = \chi/V$ $\text{m}^3 \text{ m}^{-3}$ $4\pi \text{ m}^3 \text{ m}^{-3}$
χ_g	$\chi_g = \chi_v/\rho$ $\text{cm}^3 \text{ g}^{-1}$ $1 \text{ cm}^3 \text{ g}^{-1} \hat{=}$	$\chi_g = \chi_v/\rho$ $\text{m}^3 \text{ kg}^{-1}$ $4\pi \cdot 10^{-3} \text{ m}^3 \text{ kg}^{-1}$	$\chi_g = \chi_v/\rho$ $\text{m}^3 \text{ kg}^{-1}$ $4\pi \cdot 10^{-3} \text{ m}^3 \text{ kg}^{-1}$
χ_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 ± 0.012 , and 342.5(21) stands for 342.5 ± 2.1 .