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Subvolume I 2

Sorosilicates

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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**

Table of contents

Magnetic properties of non-metallic inorganic compounds based on transition elements

Subvolume I 2: Sorosilicates

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, exchange parameter
A	%	relative area of NGR spectrum
B	T	magnetic induction
B_{hf}		hyperfine magnetic field
B, B_{eq} , B_{iso}	$Å^2$	isotropic temperature parameter
c_{ij}	Pa	elastic stiffnesses
C	emu K $f.u.^{-1}$= cm^3 K $f.u.^{-1}$	Curie constant per formula unit
C	J $g^{-1}K^{-1}$, J $mol^{-1}K^{-1}$	heat capacity
C_p		heat capacity at constant pressure
C_v		heat capacity at constant volume
C_{magn}		magnetic heat capacity
d	Å	thickness
d_{ij}	C N^{-1}	piezoelectric constant
D	cm^{-1}	Hamiltonian parameter
Dq	cm^{-1}	crystal field splitting parameter
DH	mm s^{-1}, Hz	linewidth of NGR or NMR line
e	C	electron charge
e_{ij}		strain tensor
E	Pa	Young modulus
E	V cm^{-1}	electric field strength
E	cm^{-1}	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
H		Hamiltonian
ΔH	eV	enthalpy
H	Oe, A m^{-1}	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	$Å^{-1}$	wavevector
k_B	J K^{-1}	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
Δn		birefringence
p	Pa, bar	hydrostatic pressure
p	μ_B	magnetic moment (sometimes also M is used)
p_A		magnetic moment per atom
p_{eff}		effective (paramagnetic) moment
p_M		magnetic moment per ion M
p_o		ordered magnetic moment
p_s		spontaneous magnetic moment
p_3	$C\ K^{-1}\ m^2$	pyroelectric coefficient
q	$Å^{-1}$	wavevector (also dimensionless wavevector component)
ΔQ	$mm\ s^{-1}$	quadrupole splitting
Q		order parameter
r	Å	radius, distance
$r_{M,(R)}$		radius of ion M (R)
R		reflectivity
S	$\mu V\ K^{-1}$	Seebeck coefficient (thermoelectric power)
S		spin quantum number
S	$J\ K^{-1}\ mol^{-1}$	entropy
T		transmission
T	K, °C	temperature
$T_{IC\text{-}N}$		transition temperature IC to N phase
T_{LI}		lock-in phase transition temperature
T_{ord}		ordering temperature
T_N		Néel temperature
T_t		(crystallographic) transition temperature
U_{eq}	$Å^2$	temperature parameter
υ	$mm\ s^{-1}$, $m\ s^{-1}$	velocity (mostly of absorber in Mössbauer effect)
V	$Å^3$	(unit cell) volume
V^0	deg	angle between optical axes
V_{zz}	$V\ cm^{-2}$	main component of the electric field gradient tensor
x, y, z		fractional coordinates of atoms in the unit cell
X, Y, Z		principal directions
α	cm^{-1}	absorption (extinction) coefficient
α	K^{-1}	linear thermal expansion coefficient
α, β, γ	deg	(unit cell) angles
β	bar^{-1}, Pa^{-1}	linear compressibility
β_{ij}		anisotropic temperature parameter
Γ	$mm\ s^{-1}$	linewidth of NGR line
Δcorr	cm^{-1}	effective linewidth of peaks in IR spectra
δ	ppm, $mm\ s^{-1}$	chemical shift, isomer shift
$\varepsilon = \varepsilon_1 - i\ \varepsilon_2$		dielectric constant
$\varepsilon_1, \varepsilon_2$		real, imaginary part of dielectric constant
ε_i		spontaneous strain
η		asymmetry parameter, order parameter
θ	deg	angle (bond angle, …)
Θ	K	paramagnetic Curie temperature
λ	nm, µm, Å	wavelength

Symbol	Unit	Property
λ	s^{-1}	relaxation rate (in NGR)
μ_B	$J\ T^{-1}$	Bohr magneton
ν		Poisson ratio
ν	Hz	frequency
ν_{as}	Hz	"antisymmetric" frequency
ν_s	Hz	"symmetric" frequency
ν_{OH}	Hz	frequency of O-H stretching vibration
ν_L	Hz	Larmor frequency
$\bar{\nu}$	cm^{-1}	wavenumber
$\Delta\bar{\nu}$	cm^{-1}	Raman shift
ρ	$kg\ m^{-3}$	density
ρ	Ω m	resistivity
σ	$\Omega^{-1}\ m^{-1}$, $\Omega^{-1}\ cm^{-1}$	electrical conductivity
σ	emu g^{-1} = G $cm^3\ g^{-1}$, A $m^2\ kg^{-1}$	magnetic moment per unit mass = specific magnetization
σ_s		spontaneous magnetization
ξ		order parameter
τ	s	relaxation time
χ_A	$\mu_B T^{-1}$ $atom^{-1}$	magnetic susceptibility per atom
χ_g	emu g^{-1} = $cm^3\ g^{-1}$, $m^3\ kg^{-1}$	magnetic susceptibility per gram
χ_m	emu mol^{-1} = $cm^3\ mol^{-1}$, $m^3\ mol^{-1}$	magnetic susceptibility per mole
ω	s^{-1}	angular frequency
ω_Q		quadrupole frequency

Abbreviations

ac	alternating current
apfu	atom per formula unit
AF	antiferromagnetic
c, cr	mostly as subscript: critical
calc	calculated
$CFSE^{(ex)}$	(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
μSR	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
⊥, ∥	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, $\boldsymbol{B} = \mu_0(\boldsymbol{H} + \boldsymbol{M})$ and $\boldsymbol{B} = \mu_0\boldsymbol{H} + \boldsymbol{M}$, respectively. $\mu_0 = 4\pi \cdot 10^{-7}$ Vs A^{-1} m^{-1}, A: molar mass, ρ: mass density, $\boldsymbol{P}$: magnetic moment, $\boldsymbol{M}$: magnetic moment per unit volume (magnetization, magnetic polarization).

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