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Subvolume I 3

Cyclosilicates

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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 I3 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 2005 **The Editor**

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

Subvolume I 3: Cyclosilicates

List of frequently used symbols and abbreviations

Symbols

Symbol	Unit	Property
a, b, c	Å	lattice parameters
A	cm^{-1}	hyperfine constant
A	%	relative area of NGR spectrum
B	T	magnetic induction
B_{res}		magnetic resonance field
B, B_{eq}	$Å^2$	isotropic temperature parameter
B_n^m	cm^{-1}	crystal field parameters
c_{ij}	Pa, bar, N m^{-2}	elastic stiffnesses
C	emu K g^{-1}= cm^3 K g^{-1}	Curie constant per unit mass
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
C_{ph}		phonon contribution to heat capacity
d	Å	distance
D	cm^{-1}	Hamiltonian parameter
DH	mm s^{-1}	linewidth of NGR or NMR line
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
f_{O_2}	atm	oxygen fugacity
g		spectroscopic splitting factor
G	Pa	torsional (shear) modulus
h		Planck constant
H		Hamiltonian
H	Oe, A m^{-1}	magnetic field (strength), sometimes given as $\mu_0 H$ in tesla (T))
H_c		critical field
H_{SF}		spin flop transition field
I		nuclear spin quantum number
I	various units	intensity
I_{magn}		magnetic intensity
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
K, K_T, K_H	Pa, bar, N m^{-2}	bulk modulus (K': first pressure derivative of bulk modulus)
M	G	magnetization
n		refractive index
n_o, n_e		refractive index for ordinary, extraordinary ray

Symbol	Unit	Property
p	Pa, bar, atm	hydrostatic pressure
p	μ_B	magnetic moment
p_{eff}		effective (paramagnetic) moment
p_M		magnetic moment per ion M
p_3	C K^{-1} m^2	pyroelectric coefficient
q	$Å^{-1}$	wavevector
ΔQ	mm s^{-1}	quadrupole splitting
Q, Q_{od}		order parameter
Q	$Å^{-1}$	scattering vector
r	Å	radius, distance
R	J K^{-1} mol^{-1}	gas constant
S		spin quantum number
t	s, min, h	time (delay time, annealing time, …)
T		transmission
T	K, °C	temperature
T_{max}		maximum temperature (of e.g. χ vs T plot)
T_N		Néel temperature
T_{SP}		spin-Peierls transition temperature
T_1	s	spin lattice relaxation time
υ	mm s^{-1}	velocity (of absorber in Mössbauer effect)
V^0	deg	angle between optical axes
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
δ	ppm, mm s^{-1}	chemical shift, isomer shift
η		asymmetry parameter
θ	deg	angle (scattering angle, …)
Θ	K	paramagnetic Curie temperature
Θ_D	K	Debye temperature
λ	nm, μm	wavelength
μ_B	J T^{-1}	Bohr magneton
ν	Hz	frequency, also used for wavenumber
$\bar{\nu}$	cm^{-1}	wavenumber
$\Delta\bar{\nu}$	cm^{-1}	Raman shift
ξ	Å	spin correlation length
ρ	e $Å^{-3}$	electron density (distribution)
τ	s	relaxation time
τ	deg	rotation angle (e.g. of CO_2 ribbons around ***c***-axis)
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

Abbreviations

ac	alternating current
apfu	atom per formula unit
AF	antiferromagnetic
AFLRO	AF long range order
AFMR	antiferromagnetic resonance
bcc	body centered cubic
BO	bridging oxygen
c, cr	mostly as subscript: critical
calc	calculated
CN	coordination number
CT	charge transfer
dc	direct current
1D, 2D, 3D	one-, two-, three-dimensional
DED	deformation electron density
eff	mostly as subscript: effective
emu	electromagnetic unit
exp	experimental
ECP	exchange coupled pair
ED	electron charge delocalized (doublets)
EELS	electron energy loss spectrum
EFG	electric field gradient
ELNES	energy loss near edge structure
ENDOR	electron nuclear double resonance
EPR	electron paramagnetic resonance
ESR	electron spin resonance
FTIR	Fourier transform infrared spectroscopy
FU, f.u.	formula unit
H, h, hex	mostly as subscript: hexagonal
IR	infrared
IVCT	intervalence charge transfer
L	longitudinal
LFB	low-frequency (band)
LRO	long range order
magn	mostly as subscript: magnetic
max	mostly as subscript: maximum
min	mostly as subscript: minimum
M	modulated
M	metal
MAS	magic angle spinning
MFB	mid-frequency (band)
nn, NN	nearest neighbor
nnn	next nearest neighbor
NBO	nonbridging oxygen
NGR	nuclear gamma resonance (Mössbauer effect)
NIR	near infrared
NMR	nuclear magnetic resonance
O, o	mostly as subscript: orthorhombic
ODEPR	optical detection of EPR
pfu	per formula unit
pc	polycrystal
QMC	Quantum Monte Carlo (simulation)

R	rare earth element
RT	room temperature
sc	single crystal
SP	spin-Peierls (transition)
T	tetrahedron, sometimes also for tetragermanate (type structure)
T	transverse
UV	ultraviolet
W	wadeite (type structure)
XANES	X-ray absorption near edge spectroscopy
XAS	X-ray absorption spectroscopy
XRD	X-ray diffraction
⊥, ‖	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.