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Lattice-dynamical evaluation of atomic displacement parameters of minerals and its implications: The example of diopside

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For deposit: Tables 4 through 8

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SUPPLEMENTARY MATERIAL

Table 4. Crystallographic details

System	monoclinic
Space group	n. 15 C2/c
a	9.7581(9) Å
b	8.9326(6) Å
c	5.2535(4) Å
ß	105.80(1)°
V	440.6(1) $Å^3$
Z	4
Radiation	MoKα (λ= 0.71073 Å)
Temperature	298 ± 1°
No. of reflections measured	2047 total, 971 unique
Instrument	Enraf-Nonius CAD4 diffractometer
Corrections: Lorentz-polarization; reflection averaging (agreement on I = 1.1%); empirical absorption (from 1.00 to 1.03 on I) extinction (coefficient = 2.68×10^{-5})	
Maximum 2θ	70°
h data range	-15 to 15
k data range	0 to 14
l data range	-8 to 8
Reflections included	816 with $F_o^2 > 3.0\sigma(F_o^2)$ and $\theta > 15°$
Monochromator	graphite crystal, incident beam
Attenuator	Zr foil, factor 17.5
Detector aperture:	2.0 to 3.4 mm horizontal; 4.0 mm vertical
Scan type	ω-θ
Scan rate	1 -20°/min (in omega)
Scan width, deg	0.9 + 0.350 tanθ
Parameters refined	49
Unweighted agreement factor	0.011
Weighted agreement factor	0.024
Factor including unobs. data	0.020
Esd of obs. of unit weight	1.04
Convergence, largest shift	0.22σ
Refinement	full-matrix least-squares
Minimization function	$\Sigma w(\|F_o\| - \|F_c\|)^2$
Least-squares weights	$4F_o^2/\sigma^2(F_o^2)$
High peak in final diff. map	0.5(1) e/$Å^3$
Computer hardware	80486/33

Computer software: Personal SDP (B. A. Frenz & Associates, Inc.)