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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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and its implications. An example: diopside.**

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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
β	105.80(1)°
V	440.6(1) Å ³
Z	4
Radiation	MoK α ($\lambda = 0.71073$ Å)
Temperature	298 \pm 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 $\theta > 15^\circ$
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 tan θ
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	0.22 σ
Refinement	full-matrix least-squares
Minimization function	$\sum w(F_o - F_c)^2$
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.)