08.4-05  LOW AND HIGH TEMPERATURE SPINEL (MgAl₂O₄): STUDIES ON NATURAL SINGLE CRYSTALS
(H. H. Mitchell, Ottawa, Ontario, Canada; F. Thompson, Physics Department, University of Aston
in Birmingham, England and H. P. Kay, H. H. M. Physics Laboratory, University of Bristol, Bristol, England)

X-ray-diffraction intensities have been collected from a small spherical single crystal of magnesium aluminate
spinel over half a hemisphere of reciprocal space out to sin θ/λ = 1.26 µm⁻¹ with MoKα radiation and a CAD-3
diffractometer. Almost 4000 reflections have been measured including up to 24 equivalents for general hkI
and used for a structure-parameter refinement under Fd³m symmetry, following the suggestion by Grimes (Phil. Mag.
1972 26 1217), and subsequently for refinement according to the conventionally assumed Fd³m symmetry.
The former, having an R value of less than 0.02, is found to give a significantly superior fit to the
experimental data, especially at high angles and with reflections having structure factors less than 5.0. New
and very precise atom positions and bond lengths have been calculated, which demonstrate small but significant
differences from those previously published.

The new results may lend credence to the electron

diffraction observations by Hwang, Bauer and Mitchell
(Phil. Mag. 1973 27 177) and Mishra and Thomas (Acta
Cryst. 1978 A34 678) of the Fd³m forbidden reflections
hkl with h + k + l = 4n + 2, which have been discounted as arising from double diffraction in recent work by Smith
(Phil. Mag. 1978 38 99) and by Tokonami and Morishita

08.4-07  SPACE-GROUP SYMMETRY AND STRUCTURE - PARAMETER REFINEMENT FOR MAGNESIUM
ALUMINATE SPINEL. By H. H. Mitchell, Ottawa, Ontario, Canada; F. Thompson, Physics Department,
University of Aston in Birmingham, England and H. P. Kay, H. H. M. Physics Laboratory,
University of Bristol, Bristol, England

The new results may lend credence to the electron
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(Phil. Mag. 1973 27 177) and Mishra and Thomas (Acta
Cryst. 1978 A34 678) of the Fd³m forbidden reflections
hkl with h + k + l = 4n + 2, which have been discounted as arising from double diffraction in recent work by Smith
(Phil. Mag. 1978 38 99) and by Tokonami and Morishita

08.4-06  THE SYMMETRY OF DIAMOND. By Gabrielle Donnay
and J. H. Donnay, Geological Sciences, McGill University,
Montreal, PQ, Canada, J3A 2A7.

Diamond had been assigned to point group T₃₂m by the
morphological crystallographers until Bragg and Brogg (1913)
determined its crystal structure, by X-ray diffraction, and described it in Fd³m. To this day this space group
has been accepted by the whole community. D.~i~enaver (Phil. Mag. 1978) 97 182), and subsequently for refinement
in Fd³m symmetry, following the suggestion by Grimes (Phil. Mag.
1972 26 1217), and subsequently for refinement
according to the conventionally assumed Fd³m symmetry.

The former, having an R value of less than 0.02, is found to give a significantly superior fit to the
experimental data, especially at high angles and with reflections having structure factors less than 5.0. New
and very precise atom positions and bond lengths have been calculated, which demonstrate small but significant
differences from those previously published.

The new results may lend credence to the electron
diffraction observations by Hwang, Bauer and Mitchell
(Phil. Mag. 1973 27 177) and Mishra and Thomas (Acta
Cryst. 1978 A34 678) of the Fd³m forbidden reflections
hkl with h + k + l = 4n + 2, which have been discounted as arising from double diffraction in recent work by Smith
(Phil. Mag. 1978 38 99) and by Tokonami and Morishita

08.4-08  MELANOPHILITE: COMPOSITION, THERMAL BEHAVIOR AND STRUCTURE REFINEMENT. By H. Gies
and F. Liebau, Mineralogisches Institut der
Universität, D 2300 Kiel, Germany.

Melanophilitc (M) is known as a very rare natural polymorph of silica which contains, in
addition, up to 8 percent O, N, O, N, and/or S. According to Appelmann and Kamo (Science 1965
146, 232), M is isostructural with the cubic
gas hydrates I, while Zinck (N. J. Miner. 
1973 509) reported a tetragonal superstructure.

At room-temperature mass spectroscopic analyses
of samples from four localities, we found that M contains OH, CO₂ and N₂ in varying
amounts. Under the microscope the birefringent crystals become isotropic above c. 400°C, reversibly. Although gases are lost above c. 400°C, the silica framework is maintained up to about 1175°C. An endothermic DTA peak at ca. 1475°C indicates transformation to cristobalite.

X-ray diagrams show that crystals of M are
twinned at room temperature with a tetragonal
superstructure and transform to cubic single
crystals at c. 400°C. The crystal structure of the cube, at 2000°C has been refined:

r = 13.456(3)A, Pmnm, 667 independent reflections
Robs, R = 0.061, R = 0.064. In analogy with the gas hydrates M₁₈[SIO₄]₆ tetrahedra are linked to form two types of cages: two pentagondodeca-
dehedra [Si₂] and six tetraalkalodecahedra [Si₆] per unit cell. From jobs = Scalc[Si₁₂] it is