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17.4-03 CRYSTAL STRUCURE ANALYSIS AND THE

PROBLEM OF SECONDARY MINIMA IN THE METHOD

OF LEAST SQUARES. By Richard Rothbauer, IBM

Thomas J. Watson Research Center, P. O. Box 218,

Yorktown Heights, N. Y. 10598, USA.

The problem of secondary minima restricts the

possibility of applying the cyclic refinement

algorithm of the method of least squares in

order to get ab initio solutions of physical

systems of equations, which can not be exactly

solved mathematically.

For this reason the method of least squares can

not be effectively used as a tool for ab initio

crystal structure analysis.

We will therefore here describe an alternative

to the method of least squares, which leads

approximately to the same results if the under­

lying physical problem is meaningful, but which

avoids the problem of secondary minima, be­

cause it is not based on an extremal principle.