$C_{jk} = \bar{\omega} \sum_{i=1}^{N} w_i \frac{\partial m_i(\theta^q)}{\partial \theta_j} \frac{\partial m_i(\theta^q)}{\partial \theta_k}$, where

$\bar{\omega} = (1/N) \sum_{i=1}^{N} \omega[r_i(\theta^q)/s^q]$, is a variance efficiency factor with respect to Gaussian error structure. That is the parameter estimates $\hat{\theta}$ have variances of the same order as for Gaussian samples of size $\bar{\omega}N$. The width parameter s^q is a resistant estimate constructed from residuals. Several choices are available. We use Huber's suggestion $(s^{q+1})^2 = \alpha^q/\beta$, where

$\alpha^q = \sum_{i=1}^{N} \phi^2[r_i(\theta^q)/s^q] r_i^2(\theta^q)/(N-p)$,

and β is the expected value of $Z^2\phi(Z)^2$ with Z distributed according to the true error law. For Gaussian errors $\beta = 0.72767$. The variance estimate of parameter estimate $\hat{\theta}_j$ is $s^2_{\hat{\theta}_j} = (k^2 \alpha^q \beta \bar{\omega}^2) C^{jj}$, where k is a bias correction factor defined as $k = 1 + p(1 - \bar{\omega})/N\bar{\omega}$, and p is the number of parameters in the model. With $\phi(x) = 1$, $\omega(x) = 1$, and the algorithm reduces to ordinary, non-linear, weighted least squares with classical estimates of the variances of parameter estimates. To test the robust/resistant algorithm we reanalyzed the D(+)-tartaric acid data collected in the Single Crystal Intensity Project of the IUCr [Hamilton, Abrahams & Mathieson, Acta Cryst. A26, 1 (1970)]. Comparison of three refinements, 1) a recreation of the results of Hamilton and Abrahams [Acta Cryst. A26, 18, (1970)], 2) inclusion of secondary extinction, and 3) a robust/resistant refinement for each experiment, indicates that there are strong systematic effects in most of the experiments. In the best data sets there is good agreement between extinction and robust/resistant refinements. In other experiments there is strong evidence of systematic effects other than extinction, and the two refinements differ significantly.

17.4-03 CRYSTAL STRUCTURE 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 underlying physical problem is meaningful, but which avoids the problem of secondary minima, because it is not based on an extremal principle.

17.4-04 STRUCTURE FACTOR CALCULATION OF ORIENTATIONALLY DISORDERED MOLECULES By D. Hohlwein, Institut für Kristallographie der Universität Tübingen, D-7400 Tübingen, West-Germany

The structure factor of librating or orientationally disordered molecules with gaußian distribution functions is calculated exactly by numerical integration.

The results are compared with approximation methods which correspond to a cumulant expansion of the structure factor. There are already considerable discrepancies at a libration angle of 10 degrees.

The numerical structure factor calculation has been successfully applied to the refinement of the plastic phases of C_2Cl_6 and SF_6. The half-widths of the gaußian distribution functions are 40 and 32 degrees in these cases.

The low number of parameters and their simple physical meaning are the main advantages compared to other methods like the analysis with cubic harmonic functions.

The influence of anharmonic distributions can easily be considered and is demonstrated by an example.

17.4-05 MONTE-CARLO-SIMULATION OF THE MOLECULAR DISTRIBUTION IN ORIENTATIONALLY DISORDERED CRYSTALS. By W. Prandl, Institut für Kristallographie, Universität Tübingen, D-7400 Tübingen, West-Germany.

Orientationally disordered crystals show only a few Bragg reflections. Therefore the structural information is limited. Depending on the kind of data analysis the scattering density may even become negative. On the other hand, this quantity may be calculated from the knowledge of the molecular interaction potential. In a simplifying ansatz a hard core interaction was assumed, and applied to the plastic phase of C_2Cl_6 (space group: Im3m). Because of the incompatibility between the site symmetry m3m of the molecular center of gravity and the molecular symmetry $\bar{3}$m these crystals are intrinsically disordered. In a MONTE-CARLO-procedure random orientations of a molecule and all of its eight neighbours were computed, and only configurations without atom-atom-overlap were accepted. The structure of the molecule was taken from gas electron diffraction. The results, compared with experiments obtained from neutron diffraction (P. Gerlach, D. Hohlwein, W. Prandl, F.W. Schulz, Acta Cryst., submitted) are the following. If the molecular centers are kept fixed in a bcc lattice with the experimentally found lattice constant a = 7.5 Å, then the scattering density is nearly isotropic. This is not trivial because the overall diameter of the molecule is larger than the corner-center distance in the lattice. The observed anisotropy could only be reproduced after the introduction of a random gaußian shift of the molecular centers of gravity. The amount of anisotropy is nearly independent of the a priori width $\langle u^2 \rangle$ of the gaußian, provided $\langle u^2 \rangle$ is larger than the experimental value of 0.1 Å^2.