Crystallographic Computing F R Ahmed S R Hall

international union of crystallography world list of ... *- international union of crystallography world list of crystallographic computer programs (third edition) commission on crystallographic computing chairman: members: f. r. ahmed s. a. abrahamson g. c. bassi j. s. rollett t. sakurai k. sasvari v. i. simonov ... * crystallographic computer system, and the* ***neutron scattering in chemistry. crystallographic ...*** *- crystallographic computing techniques. edited by f. r. ahmed, with co-editors k. huml and b. sedl.~,(~ek. pp. 502, figs. 134, tables 93. copenhagen: munks- ... price dkr 336.00. this book contains the proceedings of the international summer school on crystallographic computing, which was held in prague, czechoslovakia, 28 july-5 august 1975.* ***notes and news international summer school on ...*** *- school on crystallographic computing to be held in ottawa from 4 to 12 august 1969. the aims of the school will be to surveyin some detail the mathematical procedures in crys- ... f. r. ahmed, division of pure physics, national research council of canada, ottawa 7, ontario, canada. international union of crystallography report of executive ...* ***choice of scans in x-ray diffraction*** *- 144 choice of scans in x-ray diffraction expression for the optimum scanning ratio which can be easily used in practical experimental situations.* ***developments in x-ray crystallographic structure ...*** *- critically depends on crystalline order, which usu-ally deteriorates if the crystals are allowed to de-hydrate. many of the technical challenges in the* ***coordinate transformations in modern crystallographic ...*** *- application to crystallographic computing and adaptation to high-level programming languages. crystallography deals with objects defined in various coordinate systems, e.g. the fractional coordinate system (used for data or symmetry operators), the grid coordinate system* ***total synthesis of cortistatins a and j - pubss*** *- f' and f'' were those of creagh and mcauley10. the values for the mass attenuation coefficients are those of creagh and hubbell11. all calculations were performed using the crystalstructure12,13 crystallographic software package. references (1) crystalclear: rigaku corporation, 1999. crystalclear software user's guide, molecular* ***the crystallographic information file (cif): a new ...*** *- universal exchange file to be called the crystallographic information file (cif). a preliminary report on this de- velopment was presented at the xv iucr congress and general assembly (1990) in bordeaux as part of the open meetings of the iucr commissions on crystallographic data and computing.* ***hydrogen-bond distances and angles in the structures of ...*** *- 392 hydrogen bonds in amino acids and peptides side-chain donors the results are given in tables 2 and 3. three acceptors are of general importance; solvent water, the carboxyl-* ***structure determination by x-ray crystallography*** *- structure determination by x-ray crystallography i m.f.c. ladd and r.a. palmer. -- 3rd ed. p. cm. ... has access to crystallographic computing facilities, the authors can supply copies of the data used to solve the structures described in chapters 6 and 8. certain problems have been marked with an asterisk.* ***references - yale university*** *- lit - 2 hendrickson, w. a. & konnert, j. h. (1980). computing in crystallography, edited by r. diamond, s. ramaseshan & k. venkatesan. pp. 13.01 - 13.25.* ***computer program crystallographers abstracts j. appl. cryst.*** *- mission on crystallographic computing. it should not exceed 500 words in length and should use the stan- dard format given on page 189 of the june 1985 issue of the journal [j. appl. cryst. (1985), 18, 189-190]. j. appl. cryst. (1988). 21,380 crysplanes- description of the bounding faces of a poly- hedral crystal.* ***crystal structure determination: a critical view*** *- in the range 1.5 to 3 (corresponding to f/cj(f) 3 to 6, since i is proportional to f'). this has three advantages: first, the computing time necessary for refinement is reduced; secondly, the r value is reduced by elimination of those reflections associated with high a; and thirdly, the problem of how to treat reflections with* ***computer programs 459 grigg, m. w. & barnea, z. (1990). j ...*** *- tion and quality factors, such as r b, rwp, rexp, gof and the correlation matrix, can be displayed after any iteration. the computation of each profile, described by a pseudo-* ***international union of crystallography computing schools*** *- international union of crystallography computing schools james m. stewart p.o. box 472, mcconnellsburg, pa 17233-0472, usa stewart1@cvn philip e. bourne san diego supercomputer center, p.o. box 85608, san diego, ca 92186-5608, usa bourne@sdsc abstract reminiscences on iucr computing schools and their place in the overall scheme of the ...* ***applying parallel computing to quickly find the solution ...*** *- r e f i n e m e n t h a n d e d n e s s t e s t ... the dark blocks represent parallel tasks dynamically generated from various crystallographic computing programs with different parameter settings. the tasks are distributed by workflow engine to the computing facility and run parallel. upon completion, the workflow engine will harvest and ...* ***peri interactions: an x-ray crystallographic study of the ...*** *- peri interactions: an x-ray crystallographic study of the structure of 1,8-bis(dimethylamino)naphthalene* by howard einspahr,t j.-b. robert,~ richard e. marsh and john d. roberts* ***crystallographic data for: 'substituent effects on indium ...*** *- refinement of f^2^ against all reflections. the weighted r-factor wr and goodness of fit s are based on f^2^, conventional r-factors r are based on f, with f set to zero for negative f^2^. the threshold expression of f^2^ > 2sigma(f^2^) is used only for calculating r-factors(gt) etc. and is* ***crystallographic information files and report generation*** *- crystallographic information files "the acronym cif is used both for the crystallographic information file, the data exchange standard file format of hall, allen & brown (1991), and for the crystallographic information framework, a broader system of exchange protocols based* ***index to volume 55, 1970 - mineralogy, petrology and ...*** *- ahmed, e. f. r. (ed.) crystallographic computing [book review] akizuki, mizuhiko. slip structure of heated*

sphalerite albee, arden l. semiquantitative electron microprobe determination of fer 1 /fer t and mn:r /mnr' in oxides and silicates and its application to petrologic problems alberti, alberto. ***computing the mobility of grain boundaries*** *- computing the mobility of grain boundaries koenraad g. f. janssens1,2*, david olmsted1, elizabeth a. holm1, ... rely on special crystallographic anisotropies and thus have been ... limits f(r i) is a zero length vector. in these simulations, we use as ...* ***subject index to volume 55 - mineralogical society of america*** *- crystallographic computing (ahmed, e. f. r. (ed.)) li-t2 2l4l group theory and energy bands in solids (cornwell, j. f.) elastic constants 9-10 1823 landbolt-b*