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PS–02.08.16 HOW TO IMPROVE QUARTET ESTIMATES: A SIMPLE STRATEGY. By C. Giacovazzo, Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche, CNR, c/o Dipartimento Geomineralogico, Universita' di Bari, 70124 Bari, Italy; M.C. Burla[*], Dipartimento di Scienze della Terra, Universita', 06100 Perugia, Italy.

In some recent papers new attention has been devoted to the role of the quartet invariants in the phasing procedures. The main drawbacks of their use are: the strong correlation with triplet invariants and the relative weakness of the formulas estimating quartets. If triplets are estimated with high accuracy [e.g., from P10 formula (G. Cascarano, C. Giacovazzo, M. Camalli, R. Spagna, M.C. Burla, A. Nunzi and G. Polidori, Acta Cryst. , 1984, A34,278-283) or from physical measurements or from isomorphous data] then this information can be transferred into quartet estimates, which can be so evaluated with larger accuracy without any penalty in computing time. The first applications will be shown.

PS–02.08.17 NEW STRATEGIES FOR DIRECT METHODS: THE ACTIVE USE OF NEGATIVE TRIPLETS, NEGATIVE QUARTETS AND PSI-ZERO TRIPLETS. By G. Cascarano and C. Giacovazzo[*], Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche, CNR, c/o Dipartimento Geomineralogico, Universita' di Bari, 70124 Bari, Italy.

The joint probability distribution method described in two recent papers (C. Giacovazzo, M.C. Burla and G. Cascarano, Acta Cryst., 1992a,b, A48,901-906, 906-912) has been considered in order to obtain a function which is maximized by the true crystal structure. The phasing process is carried out by maximizing such a function *via* a modified tangent refinement: this implies the active use of negative triplet and quartet relationships. More recently a method has been derived (C. Giacovazzo, Z. f. Krist., 1993, 000-000) which suggests an active use of *psi-zero* triplets. These, combined with positive and negative triplets and with negative quartets, give rise

to a function which is maximized by the true structure. The theory and the applications of such a new strategy are described.

PS–02.08.18 INTEGRATION OF PATTERSON AND DIRECT METHODS: ABOUT THE USE OF INTERATOMIC TRIANGLES. By A. Altomare, C. Giacovazzo, A.G.G. Moliterni[*], Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche, CNR, c/o Dipartimento Geomineralogico, Universita' di Bari, 70124 Bari, Italy.

In some recent papers (C. Giacovazzo, Acta Cryst., 1991, A47-256-263; A. Altomare, G. Cascarano & C. Giacovazzo, Acta Cryst, 1992a,b, A48,30-36,495-500) probabilistic formulas were obtained which estimate triplet invariants given prior information on non-Harker or on Harker peaks. The formulas require prior information on the value of the interatomic vectors and on their peak intensity. It is now possible to integrate Direct Methods with a further information: the existence of interatomic triangles. The final formula estimating a triplet invariant will depend on the location of the Patterson peaks and on their intensities. Triplet phase estimates lying everywhere between 0 and 2π are allowed.

PS–02.08.19 XTAL3.2: A CRYSTALLOGRAPHIC SOFTWARE SYSTEM James M. Stewart University of Maryland, College Park MD; Sydney R. Hall University of Western Australia, Nedlands Australia; Keith D. Watenpaugh The Upjohn Co. Kalamazoo MI; Howard D. Flack University of Geneva, Geneva, Switzerland; Douglas M. Collins The Naval Research Laboratory, Washington DC; David A. Grossie Wright State University, Dayton, OH.;

Xtal3.2 package is an international development project involving about 40 researchers over a full spectrum of crystallographic interests. This development has been supported by many national and international agencies and commercial institutions since the first version in 1983. The 1992 release, Xtal3.2, contains software for 90 different calculations. These range from the processing of raw diffraction data to interactive molecular graphics, atomic charge estimation, electronic publication preparation, and the structure solution and refinement of small and macromolecules.

Xtal3.2 may be installed on any computer or OS. The standard distribution is a a single 1/2 inch magnetic tape with implementation and application documentation. A customized version is also available for PCs on disks. The versatility and portability of the Xtal package is particularly important in the increasingly common networked computing and workstation environments.