s10.m1.o5 **Monte Carlo techniques in EXPO.** A. Altomare♦, M.C. Burla*, C. Giacovazzo♦, A. Guagliardi♦, A.G.G. Moliterni♦, G. Polidori* and R. Rizzi♦, *Dipartimento di Scienze della Terra, Università di Perugia, 06100 Perugia, Italy, ♦IRMEC, CNR, c/o Dip. Geomineralogico, Università di Bari, 70125 Bari, Italy,*
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Modern Direct Methods[1] have practically solved the phase problem for small molecules when single crystal diffraction data are available. Even large structures, up to 2000 atoms in the asymmetric unit, are today quasi-routinary solved by such techniques[2]. In addition, about 400 crystal structures have been solved ab initio from powder diffraction data. In spite of this success, Direct Methods seem not able to definitively solve the phase problem for powder data[3]. This is mainly due to the collapse of the three-dimensional reciprocal space of the individual crystallites on the one-dimensional 2θ axis. Direct Methods limitations may be overcome by : a) improving the quality of the experimental data *via* high resolution experimental devices (e.g. , by using synchrotron radiation); b) exploiting the prior information eventually available on the molecular geometry. This second approach has recently opened a very active area of research, aiming at locating molecular fragments in known crystalline cells[4-5]. Structural models are postulated and randomly displaced into the unit cell according to specific algorithms. The suitability of each trial is assessed by criteria based on the agreement between the whole experimental diffraction pattern and the calculated one. We will show that a combination of Direct Methods and of Monte Carlo Techniques can routinary and completely solve crystal structures for which a smaller amount of information is available. In many minerals and inorganic structures a few heavy atoms are associated with many light atoms. Assuming that only the heavy atom positions are localized, our procedure can provide the full structure by exploiting the prior knowledge on the coordination polyedra about them. Trial structures satisfying geometrical restraints are generated and the selection of the most reliable configuration is achieved by taking into account the goodness of fit value on the profile counts. So numerous structures can be completed.

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