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ARE CRYSTAL STRUCTURES PREDICTABLE? A PROGRESS REPORT

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A workshop was held in May 1999 at the Cambridge Crystallographic Data Centre to test how well currently available programs perform when given only the atomic connectivity for an organic compound. The test was based on a selection of four compounds and eleven groups of participants , who put forward a total of 36 proposed structures. No program gave consistently reliable results, but seven of the proposed structures were close enough to an experimental structure to be classified as correct. One compound occurred in two polymorphic forms but only one of these was predicted correctly. The basic difficulty is that the calculations lead to many possible structures for each compound within a narrow energy window. Fine details of the force-fields and programs influence the energy ranking within each method. Nevertheless, present methods may be useful in providing a set of structures as *possible* polymorphs for a given molecular structure.