

Are predicted structures high pressure polymorphs?

Iain D.H. Oswald , Simon Parsons, David R. Allan and W.D.Samuel Motherwell

In 1999 and 2001 the Cambridge Crystallographic Data Centre held blind tests of crystal structure prediction. The aim of these projects was ‘...to test how well currently available methods of crystal structure prediction perform when given only the atomic connectivity for an organic compound’.

The results from the tests were fairly ‘unsuccessful’ at predicting the ambient crystal structure, except in a handful of cases. The CCDC blind tests compared the predicted structures with the experimental results obtained from certain crystallisation conditions. It is a well-known fact that some molecules can adopt many different polymorphs depending on the conditions of growth. Another technique that we have been developing in Edinburgh is the use of high-pressure as a way of accessing new polymorphs. Can we access new high-pressure polymorphs that correspond to predicted structures? Are predicted structures high-pressure polymorphs?