Structures and Phase Transitions of CuInSe₂ under High Pressure <u>Thiti Bovornratanaraks</u>^a, Varalak Saengsuwan^a, Kajornyod Yoodee^a, Malcolm I. McMahon^b, Clivia Hejny^b, ^aDepartment of Physics, Faculty of Science, Chulalonkorn University, Bangkok, Thailand. ^bSchool of Physics and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh, UK. E-mail: thiti.b@chula.ac.th

The ternary compound semiconductor CuInSe₂ has a rich variety of potential applications and has stimulated a substantial number of experimental and theoretical studies. In previous high-pressure energy-dispersive powder diffraction studies of this material, the structural phase transition from the tetragonal chalcopyrite phase to the face-centred cubic at 7.6 GPa have been reported[1]. This NaCllike structure exists up to 29 GPa, the highest pressure obtained in their experiment. We have embarked on a re-examination of the highpressure structures and transitions in CuInSe₂ using angle-dispersive powder diffraction techniques with the image-plate detector on station 9.1 at the SRS Daresbury Laboratory, U.K. We find the same structural phase transition as has been previously reported up to 29 GPa. On further compression, we have obtained extensive data through a next phase transition at 39.2 GPa. This newly discovered phase has now been identified as an orthorhombic distortion of the NaCl structure. This high pressure phase is stable up to 53.2 GPa, the maximum pressure reached for this experiment.

[1] Tinoco T., Polian A., Gomez D., Itie J.P., phys. stat. sol. (b), 1996, 198, 433.

Keywords: ternary chalcopyrite, high-pressure x-ray diffraction, diamond anvil cells