

Report on the international conferences of “The 21th Joint Seminar of the Kyushu Branch of the Chemical Society of Japan and the Busan Branch of the Korean Chemical Society” by JSPS Core-to-Core Program

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As part of the JSPS (Japan Society for the Promotion of Science) Core-to-Core Program, K. Ohyama participated in the 21th Joint Seminar of the Kyushu Branch of the Chemical Society of Japan and the Busan Branch of the Korean Chemical Society (The 21th Joint Seminar of KB-CSJ and BB-KCS) held at Pukyong National University in Busan, Korea during June 12-14, 2013. In this report, I would briefly summarize my presentation.

The 21th Joint Seminar of KB-CSJ and BB-KCS is organized by the Busan Branch of the Korean Chemical Society and co-organized by College of Natural Sciences of Pukyong National University (PKNU) and the Kyushu Branch of the Chemical Society of Japan in order to exchange scientific and technical information and to extend the collaboration between the two chemical societies.

I made a poster presentation entitled “IR spectroscopy of organic crystals having infinite double hydrogen-bond networks”. Infrared spectra of 4-amino-6-oxopyrimidine (4A6Opym) crystals indicate that intermolecular one-dimensional double-hydrogen bond chains dominate the vibrational pattern. Density functional theory calculations for a hydrogen bonded (4A6Opym)_n (n=5) oligomer reproduced the vibrational pattern of crystals. Secondary perturbation energy $E^{(2)}$ obtained by NBO analysis indicated that the H-bonding energies of double hydrogen bonds approach equivalent values with the increase in number of molecule.

