ESRF	**Experiment title:** Studies of AB_2X_2 compounds: single crystal resonant scattering diffraction of $BaZn_2Ge_2$	**Experiment number:** CH-116
Beamline: ID11-BL2	**Date of experiment:** from: 13/2/1996 to: 16/2/1996	**Date of report:** 10/2/1997
Shifts: 9	**Local contact(s):** **Åke Kvick**	*Received at ESRF:* 19 FEV. 1997

Names and affiliations of applicants (* indicates experimentalists):

Gilberto ARTIOLI *, Dip. Scienze della Terra, Univ. Milano
Davide PROSERPIO *, Dip. Strutturistica Chimica, Univ. Milano
Alessandro GUALTIERI *, Dip. Scienze della Terra, Univ. Modena
Chong ZHENG, Dept. Chemistry, Northern Illinois Univ.

Report:

Site Differentiation by Synchrotron Radiation Resonant Scattering: the Case Study of $BaZn_2Ge_2$ (1997) Chemistry of Materials, in print.

Resonance scattering was applied for the first time to the class of solids with the AB_2X_2 stoichiometry. A few members of this family seem to violate the developed rules describing the structure-property relationship, and the source of ambiguity is often the experimental determination of the structure itself. As an example, the newly synthesized $BaZn_2Ge_2$ can in principle adopt either the $ThCr_2Si_2$ or the $CaBe_2Ge_2$ type structures, and conventional diffraction techniques do not allow discrimination between the two structure models. Madelung energy and extended Hückel calculations also proved to be insensitive to the structural model. The resonance scattering method shows, however, that $BaZn_2Ge_2$ crystallizes in the $ThCr_2Si_2$ structure (I4/mmm), in agreement with theoretical analyses.

Figure 1. The possible structure aristotypes for AB_2X_2 compounds: the $ThCr_2Si_2$ type (left) and the $CaBe_2Ge_2$ type (right). Resonant scattering diffraction allowed unambiguous determination of the $BaZn_2Ge_2$ structure according to the first aristotype.