Chemical calculations are used to enhance the students’ abilities of applying chemical concepts along with the mathematical concepts to solve problems which involve numerical calculations. However, it has been found that the students’ achievement level in chemical calculations at General Certificate of Examination (Advanced Level) is considerably low. Thus, this study was aimed at investigating the problems faced by the students in chemical calculations. This is a mixed methods study. In this study question papers and interview schedules on chemical calculations were constructed and validated. Question papers were administered to a sample of 140 Grade 13 students selected from two provinces in Sri Lanka. Samples of students, teachers, and national evaluators of General Certificate of Examination (Advanced Level) were interviewed. Among other things, students’ problems in solving numerical problems in structured and unstructured formats were compared. Descriptive statistics showed that the frequency of students’ mistakes was lower in the students’ answers for the structured questions than that for the unstructured questions. Interview data reveal that most of the students have the difficulty in applying chemical concepts along with the mathematical concepts in chemical calculations.

**Keywords:** Chemical calculations, Chemical concepts, Mathematical concepts, Structured questions, Unstructured questions