

Linking Conceptual Understanding and Competency Mastery in Senior High School Chemistry: A Diagnostic Study

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ABSTRACT

This study investigated the conceptual understanding and mastery of key chemistry competencies among Grade 11 STEM learners at Pangutaran National High School. Using a descriptive quantitative research design, a diagnostic assessment aligned with the Senior High School Most Essential Learning Competencies (MELCs) was administered to fifty purposively selected participants. The assessment evaluated learners' proficiency across ten chemistry competencies, including stoichiometry, gas laws, chemical equilibrium, chemical reactions, and chemical representations. Results indicated that the majority of learners exhibited low conceptual understanding, with only one competency classified as mastered, two as nearly mastered, and two as not mastered, corresponding to the least mastered competencies. The highest-performing competency involved representing compounds using chemical formulas and structures (84%), whereas the lowest-performing competency was calculating empirical formulas from percent composition (38%). The overall mean score of 62.07% fell within the least mastered classification, highlighting widespread difficulties in integrating mathematical reasoning, conceptual interpretation, and symbolic representation. These findings are consistent with prior research indicating that learners tend to perform better in representational tasks while struggling with quantitative and abstract concepts. The study underscores the need for conceptually oriented instruction, targeted remediation strategies, and the integration of diagnostic assessment feedback to enhance chemistry learning outcomes and address persistent misconceptions.

Keywords: assessment, chemistry, conceptual competencies, senior high school, STEM,

INTRODUCTION

Education serves a pivotal role in developing learners into scientifically literate, critical thinkers capable of addressing complex, technology-driven societal challenges. Science education, in particular, equips learners to understand natural phenomena, make evidence-based decisions, and engage with environmental and societal issues. Within the core sciences, chemistry occupies a central position, explaining the composition, properties, and transformations of matter—concepts that underpin daily life, industrial processes, health sciences, and environmental sustainability (Silberberg, 2013). In the Senior High School (SHS) Science, Technology, Engineering, and Mathematics (STEM) curriculum, chemistry is intended to cultivate analytical skills and provide a foundational knowledge base for higher education and STEM careers.

Despite its significance, chemistry remains a challenging discipline for many learners. Studies indicate that students perceive chemistry as difficult due to its abstract nature, symbolic representations, and the need to navigate macroscopic, submicroscopic, and symbolic levels simultaneously (Johnstone, 1993; Taber, 2013). These challenges often manifest as low achievement, poor conceptual retention, and negative attitudes toward the subject (Chiu, 2012). Research further suggests that while learners may memorize formulas and follow procedural steps, they frequently struggle to explain underlying concepts, justify reasoning, and apply knowledge to novel contexts (Nakhleh, 1992; Nurrenbern & Pickering, 1987).

Contemporary science education emphasizes conceptual understanding over rote memorization. Curriculum reforms advocate for instructional strategies that help learners construct coherent mental models and

meaningful explanations of scientific phenomena (Bruner, 1960; Ausubel, 1968). Assessment practices are increasingly encouraged to measure reasoning and conceptual depth rather than mere factual recall. However, many classroom assessments remain focused on procedural and algorithmic tasks, leaving persistent misconceptions undetected and limiting teachers' ability to address learners' conceptual needs (Black & Wiliam, 1998).

In the Philippine context, classroom assessments indicate that high school learners often fail to achieve mastery in key chemistry competencies. Local studies report persistent misconceptions and uneven understanding, particularly in abstract topics (Balita & Padayogdog, 2020). Teachers encounter students with superficial knowledge who struggle to apply concepts meaningfully; however, these gaps are seldom systematically identified due to the lack of diagnostic assessment practices (De Leon, 2021). Diagnostic assessments offer a solution by identifying prior knowledge, misconceptions, and specific areas of difficulty before or during instruction (Nitko & Brookhart, 2014). Research demonstrates that diagnostic tools grounded in conceptual understanding reveal not only what learners know but also how and why they reason in certain ways (Treagust, 1988; Chandrasegaran, Treagust, & Mocerino, 2007). Such insights are critical for identifying least mastered competencies and informing targeted instructional interventions.

This study addresses these challenges by examining learners' conceptual understanding in chemistry using a diagnostic assessment tool. Specifically, it seeks to identify the least mastered competencies among SHS learners, providing empirical evidence to inform more effective teaching strategies, assessment practices, and learner support mechanisms.

Understanding chemistry remains a persistent challenge for SHS learners, particularly in topics that integrate macroscopic observations, submicroscopic particle behavior, and symbolic representations. Students often struggle to explain core concepts, interpret chemical representations, and apply knowledge to novel situations. These difficulties lead to misconceptions and low mastery of specific competencies, even when learners can correctly perform routine or algorithmic procedures. Conventional assessments, which emphasize factual recall and numerical problem-solving, offer limited insight into learners' conceptual understanding and fail to identify the competencies that are least mastered.

To address this gap, a diagnostic assessment tool that evaluates conceptual reasoning is necessary. Such a tool can reveal learners' misconceptions, reasoning patterns, and specific areas of difficulty, enabling teachers to target instruction effectively. This study, therefore, aims to identify gaps in chemistry conceptual understanding among SHS learners and determine the least mastered competencies to inform instructional planning, remediation strategies, and assessment practices.

Although the diagnostic assessment was designed with a conceptual orientation, the present study functions primarily as a performance-diagnostic analysis of learners' chemistry competencies. Conceptual difficulties are inferred from consistent patterns of incorrect responses across competencies rather than from direct elicitation of learners' mental models. This framing allows identification of areas of conceptual vulnerability while avoiding over-interpretation of learners' reasoning.

RESEARCH METHODOLOGY

Research Design. This study employed a quantitative descriptive research design using a diagnostic assessment approach. The descriptive component determined learners' conceptual understanding in chemistry, while the diagnostic focus identified the least mastered competencies. This design is appropriate because it evaluates learners' prior knowledge and misconceptions without manipulating variables, providing a detailed profile of conceptual understanding across selected chemistry topics.

The study was conducted at Pangutaran National High School, a public SHS offering the STEM strand, selected for its accessibility and implementation of the Department of Education's Most Essential Learning Competencies (MELCs). Participants included fifty (50) Grade 11 STEM learners enrolled in chemistry during the 2024–2025 school year. Purposive sampling was employed to select learners who were currently taking

chemistry and had prior exposure to the topics assessed. Inclusion criteria were official enrollment as Grade 11 STEM students, current enrollment in chemistry, and willingness to participate in the study.

Research Instruments. The primary instrument was a researcher-developed diagnostic assessment tool aligned with the SHS chemistry MELCs. The instrument included multiple-choice items designed to assess conceptual understanding, identify misconceptions, and determine the least mastered competencies. Content validity was ensured through review by chemistry education experts, and pilot testing was conducted to evaluate clarity, difficulty, and reliability. Revisions were made based on expert feedback and pilot results prior to final administration.

Data Gathering Procedure. Data were collected using the validated diagnostic assessment tool administered via Google Forms, ensuring accessibility and efficient data collection. Responses were automatically compiled and exported for analysis. Data were summarized using descriptive statistics, including frequency counts and percentages, to determine learners' conceptual understanding and identify least mastered competencies. Interpretation was guided by established criteria and relevant literature.

Interpretation of the data was guided by established criteria and references based on DepEd Order No. 8, s. 2015 (Table 1) as follows:

Table 2.1 Interpretation of Learners' Conceptual Understanding

Percentage	Descriptors	Interpretation
90- 100	Outstanding	Very High
85-89	Very Satisfactory	High
80-84	Satisfactory	Average
75-79	Fairly Satisfactory	Low
Below 75	Did Not Meet Expectation	Very Low

Reference: DepEd Order No. 8, s. 2015

The Mastery Levels were classified according to the percentage equivalents outlined in DepEd PPST Module 11 as shown below.

Table 2.2 Mastery Levels and Percentage Equivalent

Mastery Level	Percentage Equivalent
Mastered	80-100
Nearly Mastered	75-79
Least Mastered	51-74
Not Mastered	50 and below

Reference: DepEd PPST -Module 11

Ethical Considerations. This study was conducted in full compliance with established ethical standards in educational research to ensure the protection, rights, and welfare of all participants. Formal permission to conduct the study was obtained from the school head and the chemistry teacher prior to data collection.

Participation was entirely voluntary, and informed consent was secured after clearly explaining the study's purpose, procedures, and scope. Participants were explicitly informed of their right to withdraw at any stage without incurring any academic penalties.

No monetary or material incentives were provided to avoid any form of coercion, and participation did not influence learners' grades or academic standing. The researcher maintained objectivity and declared no conflicts of interest, holding no administrative or evaluative authority over the participants that could compromise their voluntary involvement. The diagnostic assessment instrument was used exclusively for research purposes and posed no physical, psychological, or academic risks to participants.

Confidentiality and anonymity were strictly preserved through the use of unique participant codes in place of personal identifiers. All data were securely stored and accessible only to the researcher, with proper disposal ensured upon completion of the study. Collectively, these measures ensured that the research maintained ethical integrity while providing meaningful insights to improve chemistry instruction.

RESULTS AND DISCUSSION

Learners' Conceptual Understanding in Chemistry

Table 3 presents the scores of Grade learners in the need assessment, which evaluated their conceptual understanding across different areas in Chemistry, specifically, Atomic structure, Stoichiometry, Chemical nomenclature, Chemical Reaction, and Chemical bonding. The results revealed that the learners demonstrated generally low performance across these areas, with mean scores falling below the mastery threshold.

Table 3. Learners' Conceptual Understanding

Respondents	Scores	Percentages	Interpretation
1	15	50	Very Low
2	12	40	Very Low
3	23	76	Low
4	25	83	Average
5	18	60	Very Low
6	19	63	Very Low
7	20	66	Very Low
8	12	40	Very Low
9	17	56	Very Low
10	26	86	High
11	22	73	Low
12	18	60	Very Low
13	13	43	Very Low
14	15	50	Very Low



15	18	60	Very Low
16	27	90	Very High
17	27	90	Very High
18	23	76	Low
19	19	63	Very Low
20	23	76	Low
21	18	60	Very Low
22	22	73	Very Low
23	12	40	Very Low
24	7	23	Very Low
25	27	90	Very High
26	25	83	High
27	8	26	Very Low
28	22	73	Very Low
29	12	40	Very Low
30	28	93	Very High
31	18	60	Very Low
32	11	36	Very Low
33	17	56	Very Low
34	12	40	Very Low
35	21	70	Very Low
36	12	40	Very Low
37	27	90	Very High
38	13	43	Very Low
39	21	70	Very Low
40	11	36	Very Low
41	29	96	Very High
42	17	56	Very Low
43	18	60	Very Low

44	25	83	Average
45	20	66	Very Low
46	25	83	Average
47	24	80	Average
48	21	70	Very Low
49	19	63	Very Low
50	11	36	Very Low

Legend. Very Low=below 75%; Low=75-79%; Average=80-84%; High=85-89%; Very High=90% and above

As can be seen from the table, most learners scored below the mastery threshold, with an overall mean percentage of 62.07%. Only a small proportion of learners achieved performance levels at or above the mastery criterion. The overall performance distribution reflects uneven mastery across assessed competencies.

The low scores indicate that learners struggled to recall and apply fundamental concepts from their previous grade level. These results imply that most learners entered Grade 11 with fragile conceptual foundations in chemistry. Without targeted remediation, such gaps may hinder learners' ability to cope with more advanced topics that require higher-order reasoning and representational integration. These findings underscore the need for conceptually oriented instruction and targeted remediation strategies guided by diagnostic assessment outcomes (Cooper et al., 2018; Treagust et al., 2020). Thus, strengthening conceptual understanding through diagnostic-informed instruction is essential to support learners' progression in STEM tracks.

Collectively, the results indicate that most Grade 11 STEM learners demonstrate weak conceptual understanding of chemistry. Taber et al. (2019) noted that the abstract and cognitively demanding nature of chemistry contributes to enduring misconceptions and low conceptual performance. In line with the recent literature, similar patterns have been documented in the Philippine context. Balita et al. (2020) and De Leon et al. (2021) observed that senior high school learners frequently fail to meet mastery levels in chemistry competencies requiring conceptual reasoning. These studies corroborate the conclusion that the low performance reflected in Table 3 stems from insufficient conceptual understanding rather than lack of effort.

These results reveal a clear gap between learners' motivation and their actual understanding. Without solid foundational knowledge, students are likely to face greater difficulties in advanced science courses, emphasizing the need for targeted interventions to strengthen conceptual learning.

Learners' Mastery Level of Chemistry Competencies.

Table 3.2 presents the least mastered competencies in Chemistry 10, as determined from learners' conceptual understanding scores. A total of six (10) competencies were identified: two (2) under Atomic structures, three (3) under Chemical bonding and molecular structure, two (2) under chemical nomenclature and representation, two (2) under Stoichiometry and chemical calculation and, one (1) under Gas behaviors. The high frequency of errors across items indicates that these competencies were consistently challenging for learners and were therefore classified as least mastered.

Table 3.2 Learner Performance Across Chemistry Competencies

Learning Competencies	Frequency of Error	%	No. of Correct Responses	%	Mastery Level
Recognize common isotopes and their	81	27	219	73	Nearly mastered

uses.					
Represent compounds using chemical formulas, structure formulas and models	32	16	168	84	Mastered
Name compounds given the name of the compound	66	26.4	184	73.6	Nearly mastered
Calculate the empirical formula from the percent composition of a compound	31	62	19	38	Not mastered
Calculate molecular formula given molar mass	29	58	21	42	Not mastered
Gas Laws (Boyle's, Combined, Ideal, Dalton's Law)	92	36	158	63.2	Least mastered
Draw the Lewis structure of ions	39	39	61	61	Least mastered
Write the formula of molecular compounds formed by the nonmetallic elements of the representative block	19	38	31	62	Least mastered
Draw Lewis structure of molecular covalent compound	14	29.7	33	70.2	Least mastered
Describe the geometry of simple compound	68	46.2	79	53.7	Least mastered
Mean Percentage Score	62.07				Least mastered

Legend: Not mastered (50 % below), Least mastered (51-74%), Nearly Mastered (75-79%), Mastered (80-100%)

As shown in Table 4, among the ten assessed learning competencies, only one competency was classified as mastered, two as nearly mastered, and two as not mastered, identifying the latter as the least mastered. The competency with the highest percentage of correct responses (84%) representing compounds using chemical formulas and structures was classified as mastered. In contrast, the competency with the lowest mastery level (38%) calculating the empirical formula from percent composition was identified as least mastered. The overall mean percentage across all competencies was 62.07%, which falls within the least mastered classification.

The high error rates in Gas Laws reveal learners' limited quantitative proficiency and difficulty applying mathematical models to chemical situations. Similarly, poor performance in stoichiometric tasks, particularly in empirical and molecular formula calculations, indicates weak ratio reasoning and insufficient integration of mathematical and chemical concepts. Persistent difficulties in chemical bonding and molecular structure, including Lewis structures and molecular geometry, further reflect inadequate understanding of electron distribution and three-dimensional molecular representations. These patterns are consistent with prior studies emphasizing chemistry's abstract nature and the persistence of misconceptions (Johnstone, 1993; Cooper et al., 2018; Taber et al., 2019).

In addition, performance varied across competencies, with lower scores in tasks requiring quantitative reasoning and multi-step integration. Competencies based on chemical representations, such as formulas and structures, were more easily mastered as they rely on recall and pattern recognition rather than deep conceptual reasoning (Villafañe & Lewis, 2016; Xu & Lewis, 2019). In contrast, tasks involving stoichiometric

calculations, like empirical formulas, remain challenging due to the need to integrate mathematical skills with chemical concepts (Cooper & Klymkowsky, 2018). Similar trends are observed locally, with Filipino senior high school learners showing low proficiency in quantitative chemistry tasks (Santiago & Cruz, 2023).

Overall, the results confirm that learners' mastery of chemistry competencies remains low, particularly in foundational topics essential for advanced chemistry learning, especially in areas requiring abstract reasoning and quantitative skills. This highlights the need for targeted instructional interventions that strengthen conceptual understanding, address persistent misconceptions, and provide scaffolded, context-based learning experiences to improve learners' mastery levels.

CONCLUSION AND RECOMMENDATION

This performance-diagnostic study revealed generally low mastery of chemistry competencies among Grade 11 STEM learners, with pronounced difficulties in tasks requiring quantitative reasoning and representational integration. The results indicate that learners' challenges stem from limited mathematical readiness, fragmented representational competence, and high cognitive load rather than from lack of exposure to content alone.

Instructional responses should therefore be targeted and competency-specific. For empirical- and molecular-formula instruction, explicit scaffolding of ratio reasoning, unit analysis, and mole-concept translation should precede algorithmic procedures. Representational bridging tasks that connect symbolic formulas to particulate models and macroscopic contexts should be embedded within problem-solving activities to reduce cognitive load.

Assessment practices should incorporate diagnostic items that reveal learners' reasoning pathways and common error patterns, enabling timely remediation before misconceptions become entrenched. Such targeted instructional and assessment strategies align directly with the diagnostic findings of this study and offer a practical basis for improving chemistry learning outcomes in the senior high school context.

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REFERENCES

1. Adadan, E. (2017). Using multiple representations to promote grade 11 students' scientific understanding of the particulate nature of matter. *International Journal of Science Education*, 39(5), 625–652. <https://doi.org/10.1080/09500693.2017.1294783>
2. Al-Balushi, S. M., Al-Musawi, A. S., Ambusaidi, A. K., & Al-Hajri, H. S. (2017). The effectiveness of using multiple representations in developing students' conceptual understanding in chemistry. *Chemistry Education Research and Practice*, 18(4), 681–697. <https://doi.org/10.1039/C7RP00048F>
3. Ausubel, D. P. (1968). *Educational psychology: A cognitive view*. Holt, Rinehart & Winston.
4. Balita, C. E., & Padayogdog, E. A. (2020). Conceptual understanding and misconceptions of senior high school students in chemistry. *International Journal of Science and Research*, 9(6), 1234–1239.
5. Bennett, R. E. (2018). Formative assessment: A critical review. *Assessment in Education: Principles, Policy & Practice*, 25(2), 1–17. <https://doi.org/10.1080/0969594X.2017.1415281>
6. Birenbaum, M., Kimron, H., Shilton, H., & Dori, Y. J. (2015). Students' learning outcomes from formative and summative assessment in science education. *Assessment in Education*, 22(2), 187–206. <https://doi.org/10.1080/0969594X.2014.938171>
7. Black, P., & Wiliam, D. (1998). Assessment and classroom learning. *Assessment in Education: Principles, Policy & Practice*, 5(1), 7–74. <https://doi.org/10.1080/0969595980050102>
8. Black, P., & Wiliam, D. (2018). *Inside the black box: Raising standards through classroom assessment*. GL Assessment.

9. Bretz, S. L. (2019). Evidence for the importance of conceptual understanding in chemistry. *Journal of Chemical Education*, 96(2), 193–199. <https://doi.org/10.1021/acs.jchemed.8b00733>
10. Bruner, J. S. (1960). *The process of education*. Harvard University Press.
11. Çalik, M., Ayas, A., & Coll, R. K. (2015). Investigating the effectiveness of conceptual change texts on students' understanding of chemistry concepts. *Research in Science Education*, 45(5), 683–705. <https://doi.org/10.1007/s11165-014-9442-1>
12. Chandrasegaran, A. L., Treagust, D. F., & Mocerino, M. (2017). The development of a diagnostic instrument to evaluate students' understanding of chemical reactions. *Chemistry Education Research and Practice*, 18(4), 751–768. <https://doi.org/10.1039/C7RP00025C>
13. Chiu, M. H. (2012). Identification and assessment of students' misconceptions in chemistry. *Asia-Pacific Forum on Science Learning and Teaching*, 13(1), 1–20.
14. Cooper, M. M. (2015). Why ask why? *Journal of Chemical Education*, 92(8), 1273–1279. <https://doi.org/10.1021/acs.jchemed.5b00203>
15. Cooper, M. M., & Klymkowsky, M. W. (2018). Chemistry, life, the universe, and everything: A new approach to general chemistry. *Journal of Chemical Education*, 95(4), 596–605. <https://doi.org/10.1021/acs.jchemed.7b00400>
16. Dahsah, C., & Coll, R. K. (2018). Thai grade 10 students' conceptual understanding of stoichiometry. *International Journal of Science Education*, 40(7), 797–816. <https://doi.org/10.1080/09500693.2018.1449485>
17. De Leon, J. A. (2021). Chemistry misconceptions among senior high school students: Implications for instruction. *Philippine Journal of Science Education*, 14(2), 45–58.
18. Gabel, D. L. (2016). Improving teaching and learning through chemistry education research. *Journal of Chemical Education*, 93(1), 13–23. <https://doi.org/10.1021/acs.jchemed.5b00729>
19. Johnstone, A. H. (1993). The development of chemistry teaching: A changing response to changing demand. *Journal of Chemical Education*, 70(9), 701–705. <https://doi.org/10.1021/ed070p701>
20. Kaltakci-Gurel, D., Eryilmaz, A., & McDermott, L. C. (2017). Identifying pre-service teachers' misconceptions in physics and chemistry using diagnostic tests. *Eurasia Journal of Mathematics, Science and Technology Education*, 13(6), 2799–2813.
21. National Research Council. (2016). *Developing assessments for the next generation science standards*. National Academies Press.
22. Nakhleh, M. B. (1992). Why some students don't learn chemistry. *Journal of Chemical Education*, 69(3), 191–196. <https://doi.org/10.1021/ed069p191>
23. Nitko, A. J., & Brookhart, S. M. (2014). *Educational assessment of students* (7th ed.). Pearson.
24. Nurrenbern, S. C., & Pickering, M. (1987). Concept learning versus problem solving. *Journal of Chemical Education*, 64(6), 508–510. <https://doi.org/10.1021/ed064p508>
25. Orgill, M., & Bodner, G. (2020). What research tells us about using analogies to teach chemistry. *Chemistry Education Research and Practice*, 21(2), 540–553. <https://doi.org/10.1039/C9RP00134H>
26. Piaget, J. (1972). *The psychology of the child*. Basic Books.
27. Santiago, R. T., & Cruz, J. P. (2023). Analysis of chemistry achievement of senior high school students. *Journal of Science Education Research*, 18(1), 33–47.
28. Silberberg, M. S. (2013). *Chemistry: The molecular nature of matter and change* (6th ed.). McGraw-Hill Education.
29. Sirhan, G. (2017). Learning difficulties in chemistry: An overview. *Journal of Turkish Science Education*, 14(2), 20–33.
30. Taber, K. S. (2013). *Chemical misconceptions: Prevention, diagnosis and cure*. Royal Society of Chemistry.
31. Taber, K. S. (2017). Student thinking and learning in science: Perspectives on the nature of learner ideas. *Science Education*, 101(4), 493–502. <https://doi.org/10.1002/scs.21290>
32. Taber, K. S., Akpan, B., & Ukwungwu, J. O. (2019). Challenges in learning chemistry concepts. *Education Sciences*, 9(2), 105. <https://doi.org/10.3390/educsci9020105>
33. Tan, K. C. D., & Subramaniam, R. (2020). Addressing chemistry misconceptions through diagnostic assessment. *Asia-Pacific Science Education*, 6(1), 1–19. <https://doi.org/10.1163/23641177-BJA10001>



34. Treagust, D. F. (1988). Development and use of diagnostic tests to evaluate students' misconceptions. *International Journal of Science Education*, 10(2), 159–169. <https://doi.org/10.1080/0950069880100204>
35. Treagust, D. F., & Chandrasegaran, A. L. (2020). Diagnostic assessment in chemistry education. *Chemistry Education Research and Practice*, 21(3), 715–727. <https://doi.org/10.1039/D0RP00029J>
36. Villafañe, S. M., & Lewis, J. E. (2016). Diagnostic assessment of students' understanding of matter. *Journal of Chemical Education*, 93(2), 227–236. <https://doi.org/10.1021/acs.jchemed.5b00705>
37. Villanueva, A. R. (2022). Diagnostic assessment practices in Philippine science classrooms. *Asia Pacific Journal of Multidisciplinary Research*, 10(3), 112–120.
38. Vygotsky, L. S. (1978). *Mind in society: The development of higher psychological processes*. Harvard University Press.
39. Xu, X., & Lewis, J. E. (2019). Investigating students' reasoning in chemistry assessments. *Journal of Chemical Education*, 96(5), 871–879. <https://doi.org/10.1021/acs.jchemed.8b00740>