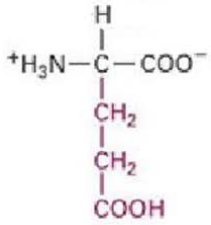
Appendix A: Structure of Amino Acids CE Prompt and Grading Rubric

Prompt and instructions to students

Write down as many **correct, distinct, and relevant facts** you can about:



Five statements will get you full credit for the problem. Recall the information you use should be information you learned in a chemistry course, including our current course. All other outside information, combined, will only count as one distinct fact towards the correct responses.

Guiding Scoring Rubric – Any five of the following possible statements result full credit

- This is an amino acid [*not distinct*: this is Glutamic acid, aka glutamate, Glu, E)
- Any indication of molecule polarity
- Classification as an acidic amino acid [possible mentioning of carboxyl group side chain]
- Any mentioning of organic functional groups present in structure (—COOH, —NH_2)
- Mentioning of chiral center, stereochemistry
- Any indication of the overall net charge of the compound (*i.e.* it's zwitterionic form/has net charge of zero/normal physiological form, etc.).
- Titration curve shows three buffer regions.
- There are three ionizable groups (protonated vs. deprotonated groups).
- Mentioning of protonation-deprotonation
- Correct drawing of ionization steps
- Listing of any pKa values (e.g., $pKa_1 = 2.2$, $pka_2 = 4.3$. $pka_3 = 9.6$)
- pI calculation (pI = (2.19+4.25) = 3.22
- Calculations of molar mass (M_r = 147.13 g/mol)
- Structure activity relationships, e.g.:
    a. References for ability to peptide bonds
    b. References to H-bonding or participation in ionic interactions
    c. Water solubility of the compound as a result of structure properties
    d. Participation in protein structure
    e. Etc.

Appendix B: Sample student responses and grading notes

Following the method of Lewis *et al.* (2011), each student response is reported in verbatim, except for statement numbering when a student did not provide one. Following each response is a quick note on how we graded the student response and thematic analysis of the student responses. The appendix provides samples from seven students whose credit in responses to structure of amino acids CE ranged from 5–2 out of possible maximum 5 points. The spectrum is provided to illustrate the varied nature of student responses.

Students A and B – Sample student response that received 4/5 credit points out of 5

Pat I - Student Responses and Grading Notes

Statement	Student A	Student B
1.	Has carboxylic acid functional group	This is in its zwitterion form
2.	acidic and charged molecule	It has a carboxyl group
3.	molecule can deprotonate & protonate	It is an amino acid
4.	amino acid can peptide bond to form a protein	It will have 3 buffer zone
5.	molecule can hydrogen bond	It can form a peptide with another copy of it self

Grading Notes:

Student A received credit for four statements as follows:

- The student received credit for statement 1 for pointing the carboxyl functional group
- The student received credit for statement 2 for classifying the compound as acidic/charged
- The student received credit in statement 3 for listing protonation-deprotonation properties
- Per the scoring guidelines, student received credit for statements 4 but not 5 owing to the distinct criteria

Student B received credit for five statements as follows:

- The student received credit for statement 1 for pointing out the overall charge of the compound
- The student received credit for statement 2 for pointing out the organic functional group present
- The student also received credit for statement 3 for identifying the structure as that of an amino acid
- The student received credit for statement 4 for pointing out the buffer regions upon titration
- And finally, student B received credit for statement 5 for invoking structure activity relationship

Pat II - Thematic Analysis of Student A's Response

- Student A statements 1 was coded as *organic chemistry concepts* for listing organic functional group.
- Student A's statement 2 classified the shown structure as acidic and charged molecule and was codes as *compound classification.*
- Student A's statement 3 was codes as *acid-base* since students deal with protonation/deprotonation during acid-base chemistry
- Student A's statements 4 and 5 were coded as *structure-activity-relationship* since the student predicted the behavior of the shown structure – the ability to peptide bond to form proteins and participate in intermolecular forces (H-bonding).

Thus,

- Responses by student A are featured under the four themes of 1) organic chemistry concepts, 2) acid-base concepts, 3) compound classification, and 4) structure-activity-relationship.
- Responses by student B are featured under the five themes of 1) acid-base concepts, 2) organic chemistry concepts, 3) structure identification, 4) titration, and 3) structure activity relationships.

Student C – Sample response that received 4 credit points out of 5

Pat I - Student C's Response and Grading Notes

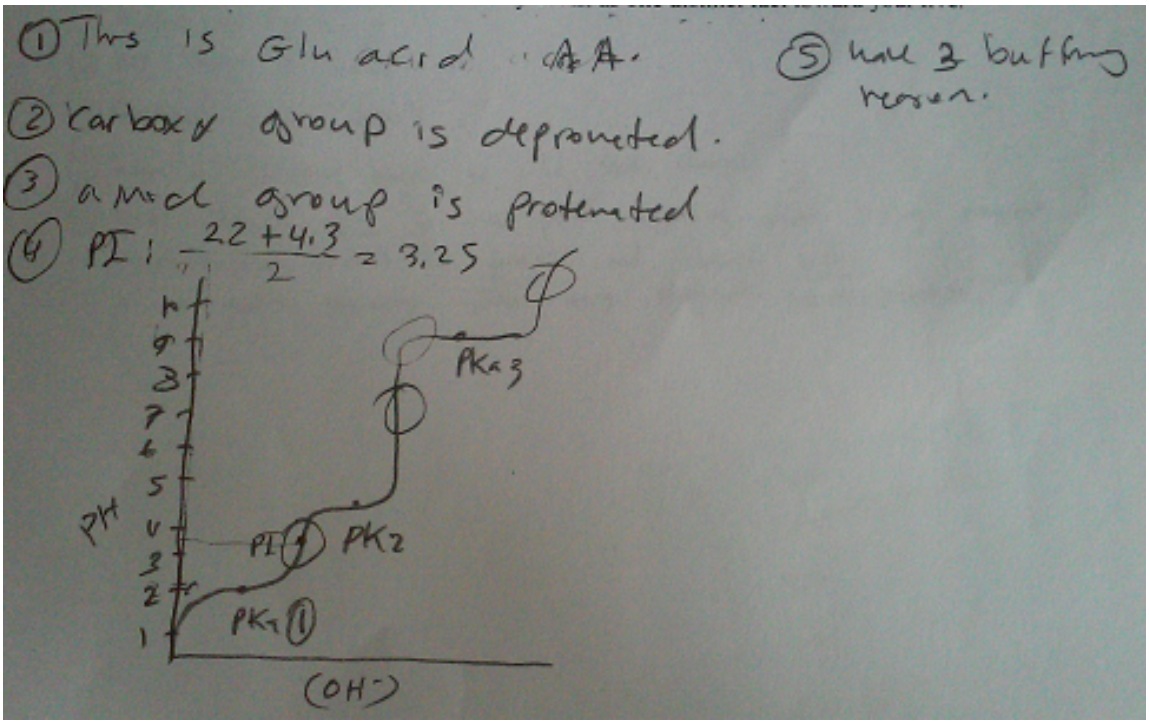


Fig. 1S Response to the structure of amino acids CE by Student C

Grading Notes:
Student C received credit for four statements as follows:

- The student received credit for statement 1 for identifying the structure shown in the prompt as that of glutamic acid
- Per the scoring guidelines, student received credit point for statements 2 but not 3 owing to the distinct criteria – both invoke protonation-deprotonation.
- The student also received credit for calculating the pI in statement 4.
- Similarly, student received credit in statement 5 for invoking buffering regions in the titration curve.

Pat II - Thematic Analysis of Student C's Response

- Statement 1 was coded as *structure identification* – identifies structure shown in the prompt
- Because statements 2-4 deal with topics often dealt with in acid-base chemistry (protonation-deprotonation, pH/pI), they were coded as *acid-base concepts*
- We made a separate category for statements such as statement 5 that specifically invoked titration concepts, consequently this statement was coded as *titration*.

Thus, the responses by student C are featured under the three themes of 1) structure identification, 2) acid-base concepts, and 3) titration.

Students D and E – Sample student responses that received 3 credit points out of 5

Pat I - Student Responses and Grading Notes

Statement	Student D	Student E
1.	It is in zwitterionic form	This is a polar amino acid
2.	This is the form it would be in under normal physiological conditions	This is an acidic amino acid
3.	This is polar acidic amino acid	This is written at physiological pH
4.	The amino group is protonated and the carboxyl group is deprotonated	This is zwitterion
5.	It has a net charge of 0	There are 3 "bumps" on the titration curve for this amino acid

Grading Notes:

Student D received credit for three statements as follows:

- Per the scoring guidelines, the student received credit for statement 1 but not 2 and 5 owing to the distinct criteria – all three describe the overall net charge of the compound.
- The student received credit for statement 3 for classifying the structure as polar and acidic.
- The student also received credit for statement 4 for mentioning protonation/deprotonation.

Student E received credit for three statements as follows:

- Per the scoring guidelines, the student received credit for statement 1 but not 2 owing to the distinct criteria – both statements classify the prompt structure as polar and acidic
- Similarly, the student received credit for statement 3 but not 4 since both describe the overall charge of the compound.
- The student also received credit for statement 5 for specific references to titration curve.

Pat II - Thematic Analysis of Student Responses

- Because student D's statements 1, 2, 4, and 5 invoke topics often dealt with in acid-base chemistry (zwitterion form/net charge and protonation/deprotonation), these statements were coded as *acid-base concepts*
- Student D's statement 4 was coded as *compound classification* – classifies prompt structure as polar and acidic
- Student E's statements 1 and 2 were coded as *compound classification* – both classify the prompt structure as polar and acidic
- Because student E's statements 3 and 4 invoke topics often dealt with in acid-base chemistry (zwitterion form and structure form at physiological pH), these statements were coded as *acid-base concepts*
- Student D's statement 5 was coded as *titration* – given the number of students who specifically mentioned titration, we created the separate code of "titration" for such statements

Thus,

- Responses by student D are featured under the two themes of 1) acid-base concepts and 2) compound classification, and
- Responses by student E are featured under the three themes of 1) acid-base concepts, 2) compound classification, and 3) titration.

Students F and G – Sample student responses that received 2 credit points out of 5

Pat I - Student Responses and Grading Notes

Statement	Student F	Student G
1.	2 carboxyl groups	This is in zwitterion form
2.	1 amino group	This is physiologically neutral
3.	amino acid	This is polar
4.	hydrophobic	This is acidic
5.		

Grading Notes:
Student F received credit for two statements as follows:

- Note, this student listed only four statements
- Per the scoring guidelines, the student received credit for statement 1 but not 2 owing to the distinct criteria – both list organic functional groups
- The student received credit for statement 3 for identifying the structure as that of an amino acid.
- The student also did not received credit for statement 4 as it is incorrect

Student E received credit for three statements as follows:

- Note, this student also listed only four statements
- Per the scoring guidelines, the student received credit for statement 1 but not 2 owing to the distinct criteria – both refer to the overall charge of the structure
- The student received credit for statement 3 but not 4, again due to the distinct criteria – both classify the structure as acidic and polar

Pat II - Thematic Analysis of Student F's Response

- Statements 1 and 2 were coded as *organic chemistry concepts* – identifies the organic functional groups of carboxyl acids and amine.
- Statement 3 was classified as *structure identification* since it simply identifies the prompt structure as that of an amino acid.
- Statement 4 is incorrect for the shown structure but coded as *compound classification* as it simply lists "hydrophobic" to describe the structure.

Thus, the responses by Student F are featured under the three themes of 1) structure identification, 2) organic chemistry concepts, and 3) compound classification.