



ELSEVIER

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Charge-transfer interaction of aspartame and neotame with several π -acceptors: Stoichiometric data



Abdel Majid A. Adam^{a,*}, Tariq A. Altalhi^a, Hosam A. Saad^a,
Amnah M. Alsuhaibani^b, Moamen S. Refat^a, Mohamed S. Hegab^c

^a Department of Chemistry, College of Science, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia

^b Department of Physical Sport Science, Princess Nourah bint Abdulrahman University, Riyadh, Saudi Arabia

^c Deanship of Supportive Studies (D.S.S.), Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia

ARTICLE INFO

Article history:

Received 25 March 2021

Revised 16 April 2021

Accepted 16 April 2021

Available online 24 April 2021

Keywords:

Charge-transfer interaction

Aspartame

Neotame

Stoichiometry

Job's continuous variation method

ABSTRACT

This data article is related to a research paper entitled "Correlations between spectroscopic data for charge-transfer complexes of two artificial sweeteners, aspartame and neotame, generated with several π -acceptors" [J. Mol. Liq. 333 (2021) 115904] [1]. Herein we present stoichiometric data of charge-transfer (CT) complexes generated from the interaction between aspartame and neotame with three π -acceptors in methanol solvent at room temperature. The investigated π -acceptors were picric acid (PA), chloranilic acid (CA), and 2,3-dichloro-5,6-dicyano-p-benzoquinone (DDQ), where the methods used to determine the stoichiometry of the CT interaction were the spectrophotometric titration method and the Job's continuous variation method.

© 2021 The Author(s). Published by Elsevier Inc.

This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>)

DOI of original article: [10.1016/j.molliq.2021.115904](https://doi.org/10.1016/j.molliq.2021.115904)

* Corresponding author.

E-mail address: majidadam@tu.edu.sa (A.M.A. Adam).

<https://doi.org/10.1016/j.dib.2021.107092>

2352-3409/© 2021 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>)

Specifications Table

Subject	Chemistry
Specific subject area	Charge-transfer (CT) complexation
Type of data	Graph/Plot
How data were acquired	OriginPro 9 software, UV/Vis spectrophotometer
Data format	Raw and analysed
Parameters for data collection	All data were collected on CT complexes generated in methanol solvent at room temperature using analytical grade chemicals.
Description of data collection	Solutions of aspartame and neotame, and each acceptor dissolved in methanol solvent were mixed and the resultant CT complexes were scanned using a UV/Vis spectrophotometer. These UV/Vis spectra were compared with those from the free donors and acceptors alone to verify the stoichiometry of the interaction.
Data source location	Department of Chemistry, College of Science, Taif University, Taif, Saudi Arabia
Data accessibility	Data are available with the article.
Related research article	A.M.A. Adam, T.A. Altalhi, H.A. Saad, A.M. Alsuhaybani, M.S. Refat, and M.S. Hegab, Correlations between spectroscopic data for charge-transfer complexes of two artificial sweeteners, aspartame and neotame, generated with several π -acceptors, <i>J. Mol. Liq.</i> 333 (2021) 115904. https://doi.org/10.1016/j.molliq.2021.115904

Value of the Data

- Investigating the charge-transfer (CT) properties of the artificial sweeteners, aspartame and neotame may be useful toward improving their uses and applications.
- Verifying the stoichiometry of the interaction between the artificial sweeteners, aspartame and neotame with different acceptors is very important to understand the mode of the interaction of these sweeteners toward improving their uses and applications.
- The most important and useful methods to determine the stoichiometry of the interaction between molecules are Job's continuous variation method and the spectrophotometric titration method. These methods are easily performed.

1. Data Description

Methanolic solutions of aspartame (Asp) and neotame (Neo) as donors at concentration of 5×10^{-4} M were each individually mixed with three acceptor solutions in methanol solvent at the same concentration (5×10^{-4} M). These acceptors were CA, PA, and DDQ. The resultant donor-acceptor systems were Asp-CA, Asp-PA, Neo-DDQ, Neo-CA, and Neo-PA, which were scanned using a UV/Vis spectrophotometer (The UV/Vis spectra dataset were provided as separated Excel sheet). The stoichiometry of the interaction between the donors (Asp and Neo) and the acceptors (CA, PA, and DDQ) was obtained using i) Job's continuous variation method [2], and ii) the spectrophotometric titration method [3]. Fig. 1(a-e), respectively, contain the curves generated for the five systems using Job's continuous variation method (the raw data associated with this figure were based on one measurement, and listed in Table 1). Fig. 2(a-e), respectively, contain the curves generated for the five systems using spectrophotometric titration method (the raw data associated with this figure were based on one measurement, and listed in Table 2).

2. Experimental Design, Materials and Methods

2.1. Materials

Analytical-grade Asp ($C_{14}H_{18}N_2O_5$; 294.30 g/mol; purity $\geq 98\%$), Neo ($C_{20}H_{30}N_2O_5$; 378.47 g/mol; purity $\geq 98\%$) were bought from SUPELCO Analytical Company. PA ($C_6H_3N_3O_7$; 229.10 g/mol; purity $\geq 98\%$), CA ($C_6H_2Cl_2O_4$; 208.98 g/mol; purity $\geq 98\%$), and DDQ ($C_8Cl_2N_2O_2$; 227.00 g/mol; purity 98%) were bought from Sigma-Aldrich Chemical Company.

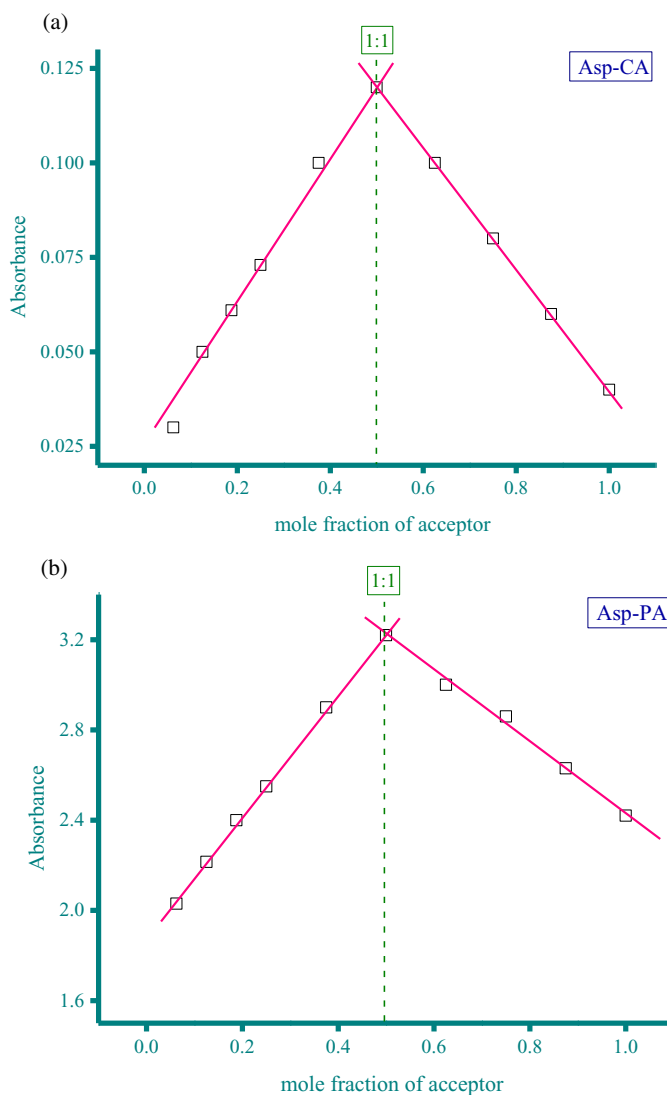


Fig. 1. a. Composition between Asp and CA determined by Job's continuous variation method. b. Composition between Asp and PA determined by Job's continuous variation method. c. Composition between Neo and DDQ determined by Job's continuous variation method. d. Composition between Neo and CA determined by Job's continuous variation method. e. Composition between Neo and PA determined by Job's continuous variation method.

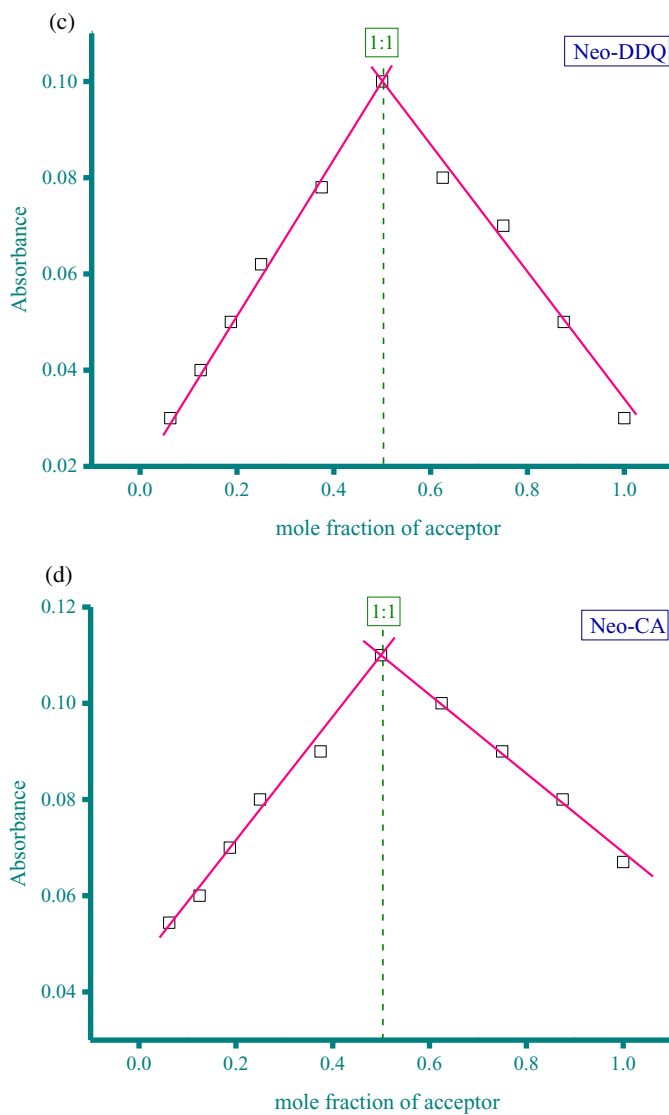


Fig. 1. Continued

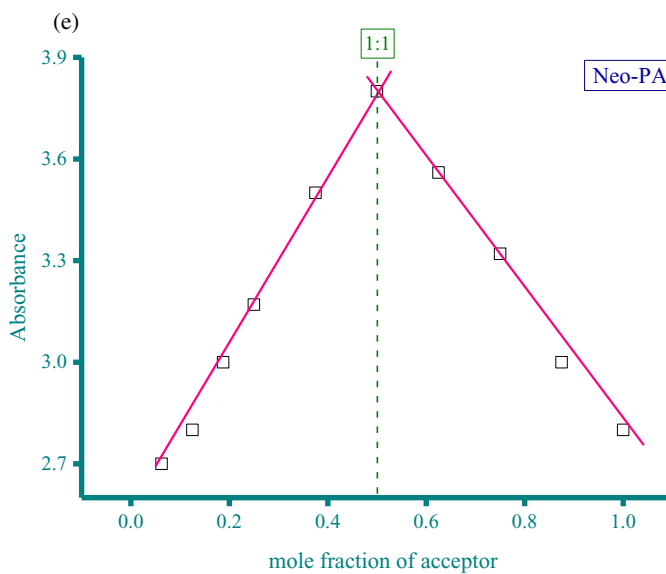


Fig. 1. Continued

Table 1

Absorbance of the Asp-CA, Asp-PA, Neo-DDQ, Neo-CA, and Neo-PA systems at different mole fraction of acceptor (the raw data for Fig. 1).

Mole fraction of acceptor	Absorbance				
	Asp-CA	Asp-PA	Neo-DDQ	Neo-CA	Neo-PA
0.0625	0.03	2.03	0.03	0.0544	2.7
0.125	0.05	2.215	0.04	0.06	2.8
0.1875	0.061	2.4	0.05	0.07	3
0.25	0.073	2.55	0.062	0.08	3.17
0.375	0.1	2.9	0.078	0.09	3.5
0.5	0.12	3.22	0.1	0.11	3.8
0.625	0.1	3	0.08	0.1	3.56
0.75	0.08	2.86	0.07	0.09	3.32
0.875	0.06	2.63	0.05	0.08	3
1	0.04	2.42	0.03	0.067	2.8

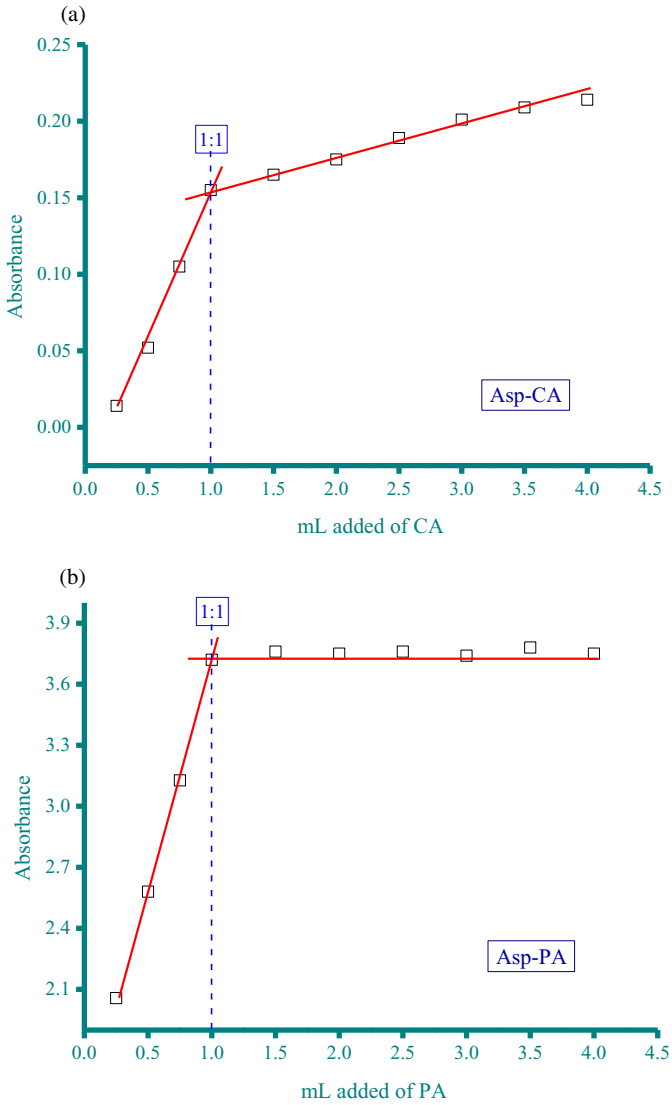


Fig. 2. a. Composition between Asp and CA determined by spectrophotometric titration method. b. Composition between Asp and PA determined by spectrophotometric titration method. c. Composition between Neo and DDQ determined by spectrophotometric titration method. d. Composition between Neo and CA determined by spectrophotometric titration method. e. Composition between Neo and PA determined by spectrophotometric titration method.

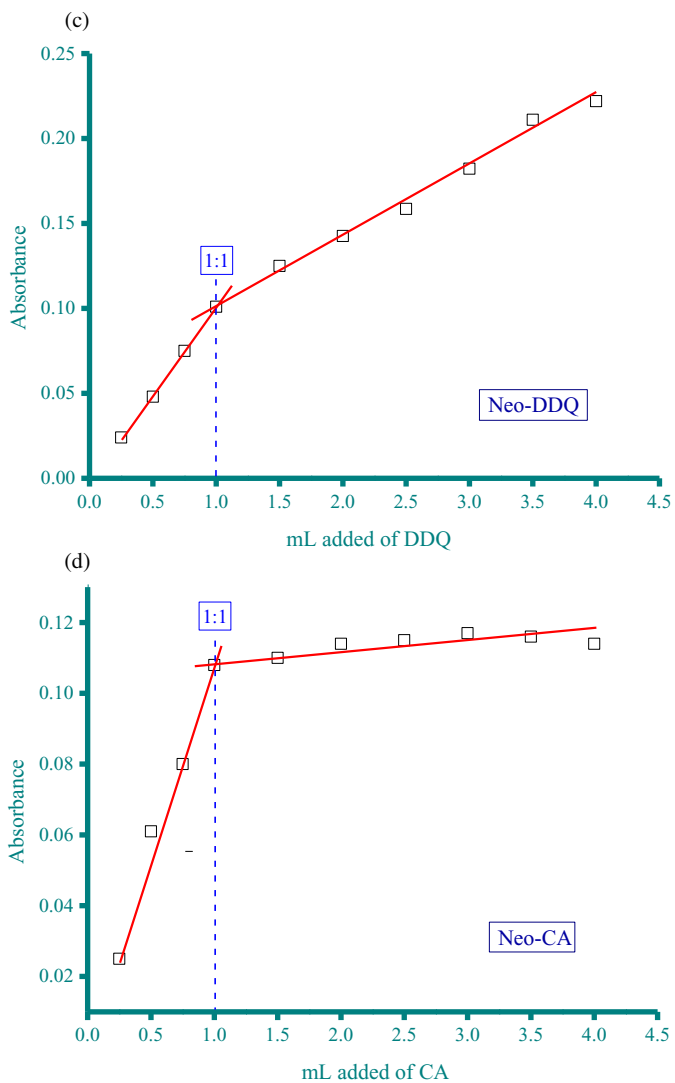


Fig. 2. Continued

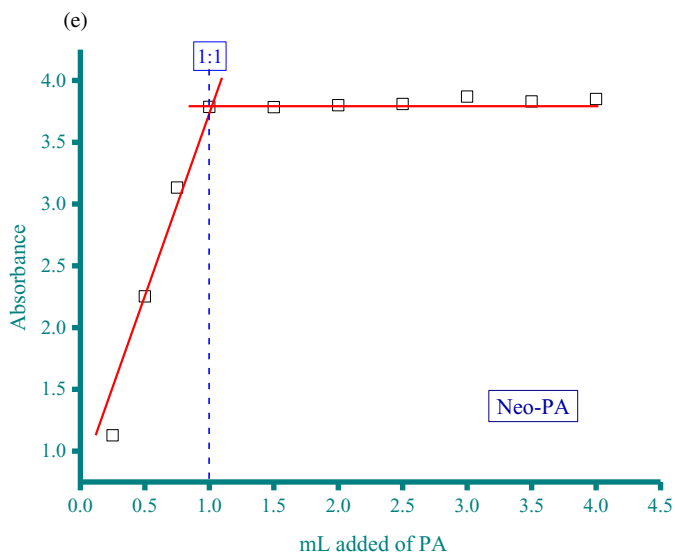


Fig. 2. Continued

Table 2

Absorbance of the Asp-CA, Asp-PA, Neo-DDQ, Neo-CA, and Neo-PA systems at different acceptor volume (the raw data for Fig. 2).

mL added of acceptor	Absorbance				
	Asp-CA	Asp-PA	Neo-DDQ	Neo-CA	Neo-PA
0.25	0.014	2.057	0.024	0.025	1.128
0.5	0.052	2.58	0.048	0.061	2.252
0.75	0.105	3.127	0.075	0.08	3.133
1	0.155	3.72	0.101	0.108	3.786
1.5	0.165	3.76	0.125	0.11	3.784
2	0.175	3.75	0.1426	0.114	3.8
2.5	0.189	3.76	0.1586	0.115	3.81
3	0.201	3.74	0.1822	0.117	3.87
3.5	0.209	3.78	0.211	0.116	3.83
4	0.214	3.75	0.222	0.114	3.85

2.2. Methods

1. Donors (Asp, Neo), and acceptors (PA, CA, and DDQ) solutions were individually prepared at 5×10^{-4} M in methanol in 25-mL volumetric flasks.

2. The solubilized donor (Asp or Neo) (1 mL) was combined with each solubilized acceptor (PA, CA, or DDQ) (1 mL) and methanol (3 mL) in 5-mL glass tubes to generate the Asp–CA, Asp–PA, Neo–DDQ, Neo–CA, and Neo–PA systems.

3. The UV-visible spectra of the free compounds and prepared systems were collected at room temperature from 200 to 800 nm using a Perkin–Elmer Lambda 25 UV/Vis spectrophotometer and used to obtain the CT band (λ_{CT}).

4. To verify the stoichiometry of the interaction between donors and each of the acceptors using the spectrophotometric titration method, the absorbances (λ_{CT}) of 10 standard solutions with varied donor to acceptor molar ratios (from 4:1 to 1:4) were plotted against the volume of the acceptor in each standard solution.

No. of the standard solution	1	2	3	4	5	6	7	8	9	10
Molar ratio (donor: acceptor)	4:1	2:1	1.3:1	1:1	1:1.5	1:2	1:2.5	1:3	1:3.5	1:4
Volume of the acceptor (mL)	0.25	0.5	0.75	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Volume of the donor (mL)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

5. To verify the stoichiometry of the interaction between donors and each of the acceptors using Job's continuous variation method, the absorbances (λ_{CT}) of 10 standard solutions with varied molar fractions of donor and acceptor ($C_{donor} + C_{acceptor}$) were plotted against the molar fraction of the acceptor in each standard solution.

No. of the standard solution	1	2	3	4	5	6	7	8	9	10
Molar fraction of acceptor	0.0625	0.125	0.1875	0.25	0.375	0.5	0.625	0.75	0.875	1.0
Volume of the acceptor (mL)	0.25	0.5	0.75	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Volume of the donor (mL)	3.75	3.5	3.25	3.0	2.5	2.0	1.5	1.0	0.5	0.0

CRediT Author Statement

Abdel Majid A. Adam: Data curation, Writing – original draft, Writing – review and editing; **Tariq A. Altalhi:** Conceptualization, Methodology, Software, Supervision; **Hosam A. Saad:** Visualization, Investigation, Software, Validation; **Amnah M. Alsuhaibani:** Visualization, Investigation, Software, Validation; **Moamen S. Refat:** Conceptualization, Methodology, Software, Supervision; **Mohamed S. Hegab:** Visualization, Investigation, Software, Validation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could be perceived to have influenced the work reported in this article.

Acknowledgments

This work was funded by Taif University Researchers Supporting Project Number (TURSP-2020/02), Taif University, Taif, Saudi Arabia.

Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:[10.1016/j.dib.2021.107092](https://doi.org/10.1016/j.dib.2021.107092).

References

- [1] A.M.A. Adam, T.A. Altalhi, H.A. Saad, A.M. Alsuhaibani, M.S. Refat, M.S. Hegab, Correlations between spectroscopic data for charge-transfer complexes of two artificial sweeteners, aspartame and neotame, generated with several π -acceptors, *J. Mol. Liq.* 333 (2021) 115904.
- [2] K.S. Kumar, T. Parthasarathy, *J. Solut. Chem.* 46 (2017) 1364.
- [3] D.A. Skoog, *Principle of Instrumental Analysis*, Third ed., Saunders, New York, USA, 1985 (Chapter 7).