

Ma a ca Mode o Ca a e ene a on a yd o e
ono p a enbe e y epa en o Ma a c

Abstract

Beck e o a a en be o nd d a a a epobe a a d e o
po n e o d ea e c a a a e a ed ca need o e ec e ca a e
e ene a on p o a a de e op en o app a cond on a n o
b o o ca y e e ce an cond on n ab n p o ec e p e en and d a
a a ca ode o ca a e e ene a on a yd o e aboco pa be ca od n
ae a p no e ode p e en ed n o a de ned o be o e b o o ca n
na e anpe o ode

Ca a e a connec e e a con an pec a ce (and ocy e) and
d nd n on a e a o a p ace n a a y en on en c ond ocy e a e ab e o
epa no da a e b o e ex en e da a e can ende a ca a e epa ab e by
na a e an Con e en y e e ac a e e e ncy e e ode e a y e o
o d na y d e en a e a on a a e e b d p o ex ace a a x
(CM) a e c a a e a o ca a e n yd o e o a e epa

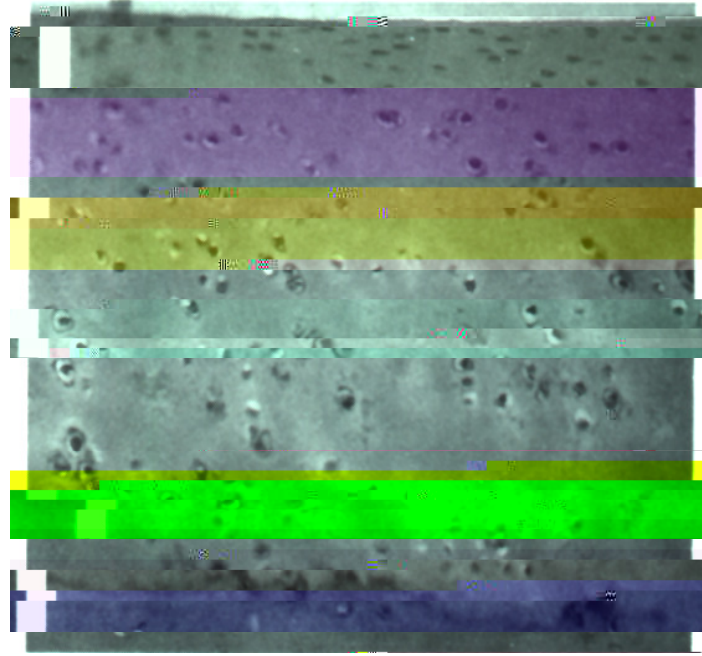
Introduction

p a o e o a on a a ca a e a d nd on y n on p

ce ... ond ocy e co p eony^r o ... ca a e o^u e^r ee (00)

u e^r ... ca a e u e ca eed ... ond ocy e No e ...
c ond ocy e a eno n con ac ... ac ... aed pe ed ... CM
p ... ond ocy e po d ce ... CM ... o o ... non- ... ae o^u e n
ca a e (Mod ... 00)

u e^r Ca a e p u e



u e^r ... ca a e u e No e ... ond ocy e (da po) a e
d pe ed ... CM p ... ce ae^v pon be o b d n and an an n
... CM (NC ...)

p ... CM e ... ade o ... o co ponen co a en and p o eo y an
App ox ae y 0 o ... dy e ... ca a e ... ade o co a en ... ee
00) Co a en o ... on ope- e u e^u e ... ade o a no ac d c an (Mod ...
00) - ... e“ ope ... a ... ca a e ab y o e c and o e a e ... ee
o ce ... ee (00) p ... co a en o e e ... e e a e yn ... zed on
bo o e a ac ed o ... endop a c e & u ... (...) (... ond ocy e) o
nd ... a a no ac d u ... p o ce n o e e n ... and Go appa d and
co a en and ... a ed p o co a en a ... p o n) a e ec eed o ... ce

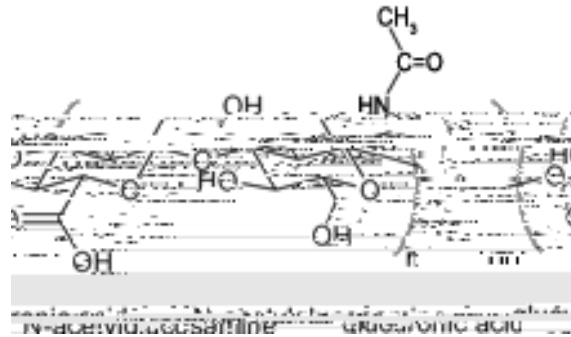
te ond ocy e) nce 6 de ace a and co - n o n aco a en

ne o 6 od h 00) Co a en n a CM p c d ed n u e

u e Co a en and P o eo ycan n CM

u e aco a en and p o eo ycan and a co p e CM
p a en e pon be o e c n en b ca a e and
p c d ed a e e b p a p o eo ycan e h a n a e

U e yal onan u cl e



U e o c a u cl e o n e n o yal onan
 yal onan u a bac bone o e p o e o ycan o e e
 p // yco an co / a yal onan)

yal onan ade by an enzy e (A yn a e) n c ond ocy e ce
 e b ane and ed a e y an po ed o ce Nex a yal onan
 a ac ed (a a n e p o e n) o a e can A e an con o aco e p o e n
 (yn a zed on a) a ac ed o c ond o n u ae and e a n u ae u a +c an
 a a e added n a Go) A e can en ce e ed p u a na p o e o ycan
 u cl e e e be a "cen pede eon n o a yal onan o e e (body) a ac ed
 o u p e co e p o e n (e) eac o u h a e u p e u a o p (e e)
 (od h 00) U e u ae h u cl e

U e P o e o y c a n S u c l e

U e o o p o e o y c a n a e c o p o e d o y a l o n a n c o e p o e n a n d
U a - U a e o p e o n d o n U a e a n d e a n U a e) P e n e a e
c a e o n e e o e e e p o d a a e o e p o e o y c a n
P o n a p e d / o y n a b o c e r / e e e)

e a p o e o y c a n o e e e a e a n b e o n e a e c a e o n e
a a c n a e e o d e 00 "A e a C a a e 00) A a e U e y-
p e c e n o e c a a e e a e p e a b y o d a a e n o e c a a e
p o a n o a e a o e a o n b e c k e e d e a e c a a e a b e
e a n d c o p e o n o c e e e 00 "A e a C a a e 00) P e
n U x o a e a o a o e d U o n o

prode ca ecan co pex A ecan en eac ... yal onan o o ...
co peepo eo ycan n ... e ... eboo ca poce e

U e C ond ocy e P od c on o CM



Collaps (CI)

U e ... a d co pond p od ced by ac ond ocy e
n en d U e no ace ... ace a e d co pond ... en U a
U ae ... coepoen co a en and yal onan poce e ... and) p U a
U ae and coepoen co b ne o o a ecan poce) na y yal onan and
a ecan co b ne o o ... co peed po eo ycan poce)

n n

enca a e da a ed ... e o n U yo d ea e) ... e e e e a
ob ace o epa ... e no a ... den yo c ond ocy e nca a e o o
... ca a e CM (See U e r) Any da a e a de oy c ond ocy e ean
... e e e en e e o ... o an an ... ca a e p ... co pond ed by ... ac
... c ond ocy e oo e ... ab yo ... o ca yd de ... e ne c ond ocy e can be
... ade) and c ond ocy e a eady ... a e a ... ed na U a ab yo epa de ec ... na y
ca a e ac bood e e o n en U d U e o ... ce ... n ... a
o a on o ca a e bood a a ab e o ... c ond ocy e ... da a ed a U e

ca a e e e e blood ... pond n ... en e c) no a a a ab e o
a ... hepa ... ee ... 00) A a e u o ca a e' ed na a ab y
o ca n a n u e e e ab p on e nee) can ca ... e a e da a e e
po n u y a ...) canno

yd o

Beck e o e ed ab yo ca a e o epa e ed ca ec n e a e
ben de e oped o ac a e e ca n poce ne u c ec n e n o e u ca y
open n e n u y e nec n yd o e o e ca y and en c n
ca a e/ u e/e c bac o e e e e e 00) Spec ca y yd o e con
o ya onan eeded ... ond ocy e o an ex e na e ce) ya onan e
bac bone o p o e o y can and a o ab e o b nd a e u exp ann e e
con ency o e yd o e p e an dea e e ond ocy e de e n n
e e n a n) e ya e no n ca a e e ben o p od ce e CM p e
yd o e e e a ab oco pa be ca od eep n e e ond ocy e paced e e
e n u y e and p o d n o e n a u c u e o e e a e can be e p e
ca a e be e ab e o e a e e ca od n p ace en a n o a od nepea e e (m)-0

p̄ ẽ nde yn a 4 p on ẽ a ẽ ode ep e en one ce (ẽ and ocy e)
 ẽ h ẽ an "a ned ẽ o ẽ ca a e o epa p̄ ẽ n 4 y con de ed o be
 ẽ a ed ẽ n ẽ ce a ned o ẽ e (M ẽ) ẽ e 4 ab y a o ẽ o ẽ ce
 n ẽ n 4 y e ẽ e ed ẽ o ẽ e a ẽ) p̄ ẽ h ode ẽ a ẽ a ab e
 co e pond n o a 4 e (ẽ n ed) ẽ CM (M) n ẽ a ned o ẽ e ono e c
 ẽ n n ed) ẽ MC (M) yd o e (ẽ) and ẽ n ẽ n de one a e a e ce (ẽ)
 a ab e a eno a zed o ce an e e ence a ẽ n (ẽ e ẽ n ẽ a eno a zed
 o ẽ n a 4 a e e o ẽ ba e ne ẽ n a ẽ n ẽ any ẽ a abo e ẽ
 4 ed o epa ẽ ca a e p̄ ẽ n ed a x on ẽ o ẽ and no a zed o ẽ
 dea ẽ CM concen a on and o ẽ ep e en ẽ a e ẽ a y e e) By con en on ẽ
 ẽ n a e a ed a ẽ ẽ e e ẽ eno epa o ẽ n ẽ ca y ca a e M
 ẽ and ẽ M 0 ẽ da a ed ca a e o e e M < ẽ and yd o e n e ed no
 ẽ de ec ẽ n ẽ 0 ẽ a ode abo e ẽ n a c o ẽ e ene a on co e
 o ẽ n ẽ en e 4 a on (ẽ 4 a on) M < ẽ ẽ n ẽ n ẽ concen a on n e ea e
 (ẽ ẽ ce en n no n ẽ ca y ca a e a o ẽ e n ẽ n no ẽ ce) p̄ ẽ
 ẽ n concen a on o e ed a M p od ced M concen a on n e ea e ẽ n
 ẽ abo e ẽ (ẽ a een o ẽ e n ẽ a on ẽ) Nex ẽ e ac ẽ ca
 eac on be ẽ en ẽ n n ed a x M and ẽ yd o e ẽ 4 o n n ed
 a x M p̄ ẽ h eac on e appea a ẽ a e n ẽ e o ẽ e 4 a on
 (ẽ 4 a on) p̄ ẽ e e 4 a on ẽ e n ẽ e ca y o ed ẽ n Ma ẽ a ca (ẽ e
 append x o no eboo) o e 0 o 00 p̄ ẽ n a cond on ẽ e e ẽ 0 M

o n Mod

The above is a code for the purpose of the analysis of the data. The code is composed of the following parts:

 1. The first part is the name of the variable being measured.

 2. The second part is the unit of measurement.

 3. The third part is the scale of measurement.

 4. The fourth part is the type of measurement.

 5. The fifth part is the source of the data.

 6. The sixth part is the date of measurement.

 7. The seventh part is the location of measurement.

 8. The eighth part is the name of the researcher.

 9. The ninth part is the name of the institution.

 10. The tenth part is the name of the project.

 11. The eleventh part is the name of the sponsor.

 12. The twelfth part is the name of the funding agency.

 13. The thirteenth part is the name of the grant number.

 14. The fourteenth part is the name of the investigator.

 15. The fifteenth part is the name of the principal investigator.

 16. The sixteenth part is the name of the co-investigator.

 17. The seventeenth part is the name of the advisor.

 18. The eighteenth part is the name of the committee member.

 19. The nineteenth part is the name of the chairperson.

 20. The twentieth part is the name of the secretary.

 21. The twenty-first part is the name of the treasurer.

 22. The twenty-second part is the name of the member at large.

 23. The twenty-third part is the name of the member at large.

 24. The twenty-fourth part is the name of the member at large.

 25. The twenty-fifth part is the name of the member at large.

 26. The twenty-sixth part is the name of the member at large.

 27. The twenty-seventh part is the name of the member at large.

 28. The twenty-eighth part is the name of the member at large.

 29. The twenty-ninth part is the name of the member at large.

 30. The thirtieth part is the name of the member at large.

Mod o d oo

The code is a sequence of characters that represent the data. The code is composed of the following parts:

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Nu → Cl, H, S, P

P + S → PS

PS + H → X

dea y ene ode da o ae o e e od o ode n ea yca ae
 n en da a ea e and n ca ae e pond ae da ae
 na y ode d ae a " u cu a te od p ca ae need oe
 n a a on o u cu e node obe abe o ca u cu e co d be ed
 by ea on o po eo ycan co a en ya onan o o eco bna on ae o)
 Abo e te od a nu yo ae nu y yd oe nec on) ca ae
 d ea b be o te od sa e nu y yd oe nec on) ca
 ca ae dno ea

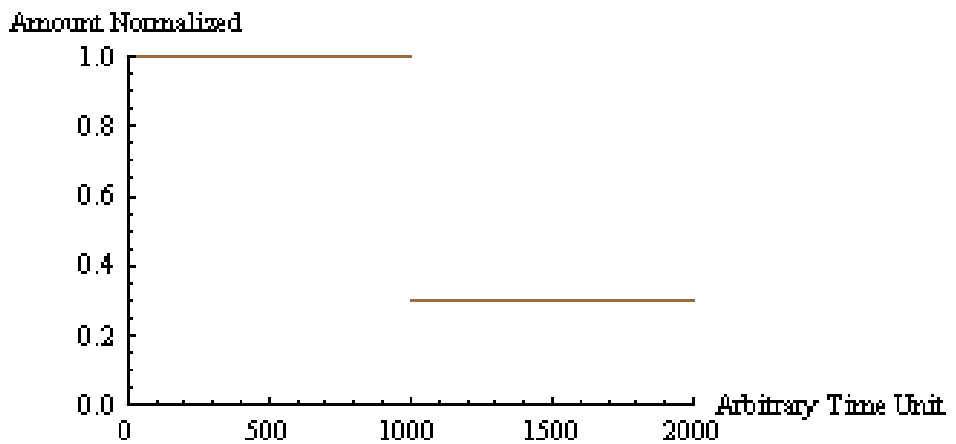
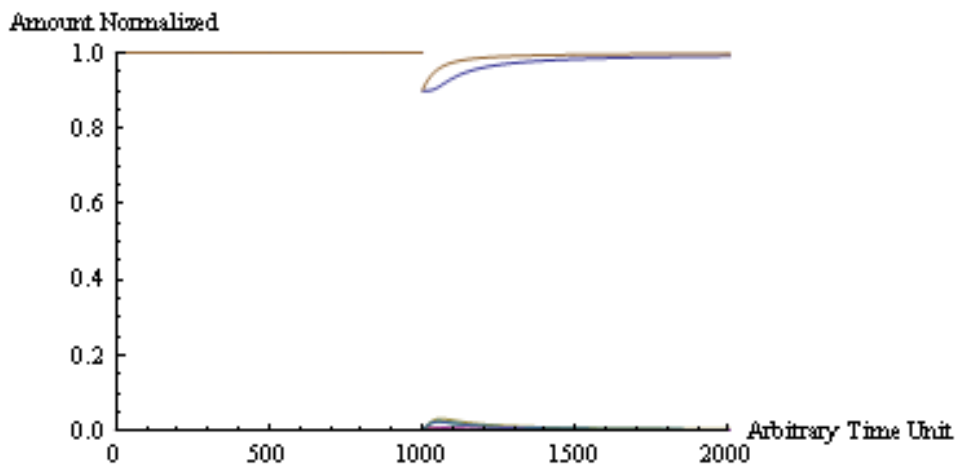
Mod y of on

n abo e pec ca on o o n ode a ceaed

e ... o co ... de c bed abo e ... a on (so a en) nc ea e ... an
 nc ea e n ... en b ... n b ed a co a en p od ced (C e) ... a on
 (ya l onan) nc ea e ... an nc ea e n ... en b ... n b ed by o a on o
 p o eo ycan and ya l onan A eac on e be een a ecan (S) and ya l onan
 (e o e ya l onan o a y e ... a on (so e p o en) nc ea e ...
 n ... n b ed by co e p o en and p o eo ycan o a on and dec ea e by a
 eac on e be een co e p o en and u a u ae ... a on o o a a
 o c o ... a on excep ... u a u ae n ead o co e p o en ... a on
 (a ecan) nc ea e ... a eac on e be een co e p o en and u a u ae
 n b ed by o a on o a ecan and dec ea e by a eac on e be een
 a ecan and ya l onan na y e ... a on (p o eo ycan) nc ea e ... a eac on

ep e en a n can n^u y o e ca a e G ap ta o^u on o e e o^u n
 appea n u e

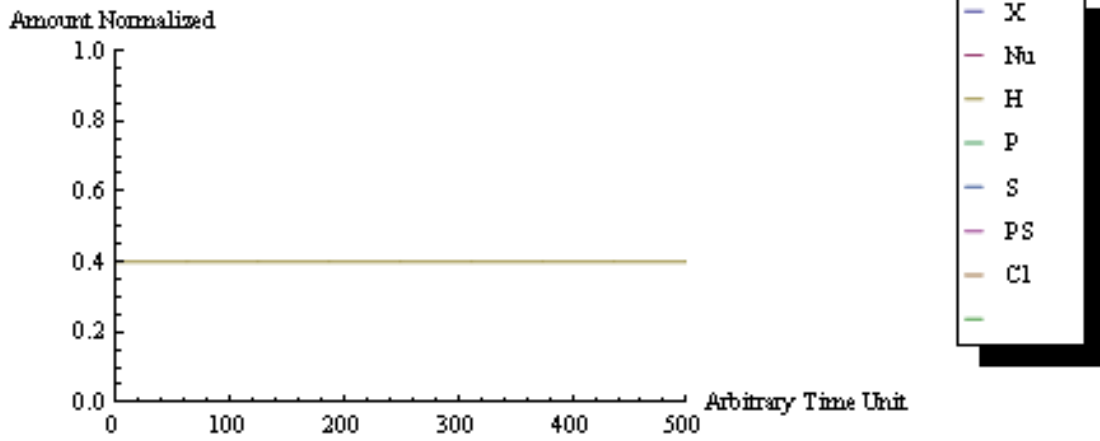
u e P a a e n ced o e a y Ca a e



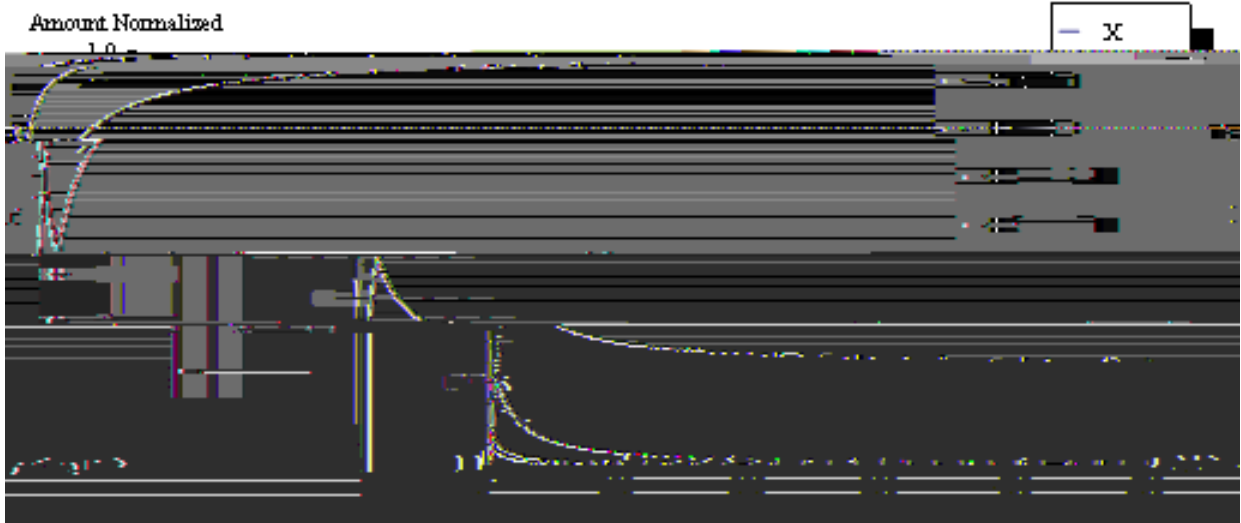
u e o o^u on o e e a on e da a e (0^r and 0 e pec e y)
 a n ced on e ca a e p a n^u y o e a e 000 and can be een by e
 p do n n e co a en and p o e o y can e e n bo h ap h p e ca a e a
 a be o e e n e n n a n ce a can be een by e n e a e n p o e o y can and
 co a en e e p e p o e o y can e e o a be n d e co a en p h c o d be e
 e o e p a e a co e cen a e e e d o e a c a o e n e d a e a e
 e d o e p o d c on o e p o e d y can n e o d e No e n e o p ap h a
 e n and o e n e d a e " c - o n - n e p o n e o e da a e (een by e
 a " p a e bo o o e ap h n e e cond ap h e ca a e a no
 a be o e e e a can be een by e a n e a o e co a en and p o e o y can)

Hydrogenation of a polyacetylene chain

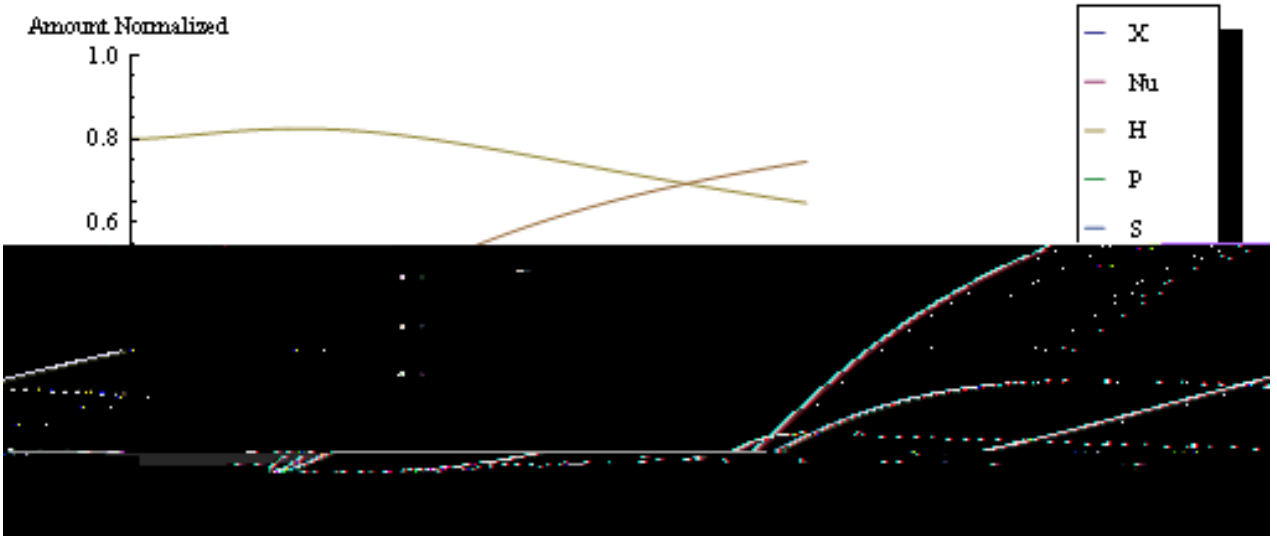
(a) (continued)



(b) (continued)



(c) (continued)

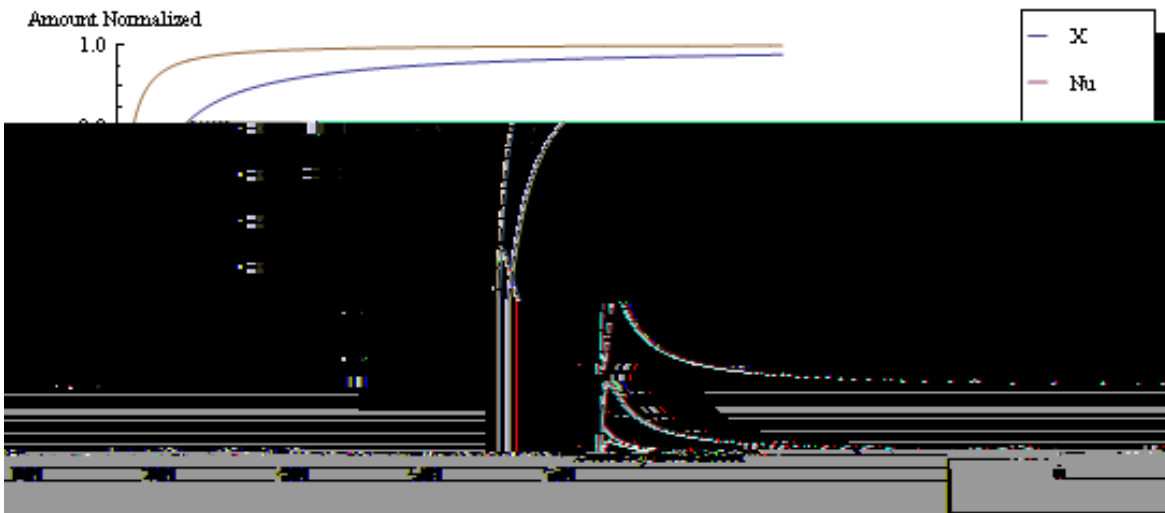


U e ϕ da a ed ca a e e pond ϕ yd o e nec on n ϕ
 po 0 ya onan ϕ nec ed ϕ no end ϕ ca ca a en ϕ
 n ance ϕ ya onan ϕ e ay a 0 and co a en ϕ and
 po eo ycan ϕ e e ay a 0 n ϕ econd po 0 ya onan nec ed ϕ
 end ϕ ca ca a e a can be een by ϕ n ca e o co a en and
 po eo ycan o ad ϕ a ϕ ne ed a e a e a o p od ced and ϕ ed a can be
 een n ϕ econd and ϕ d po a ϕ b ance ϕ a pea and ϕ n co e bac do n
 o ze o

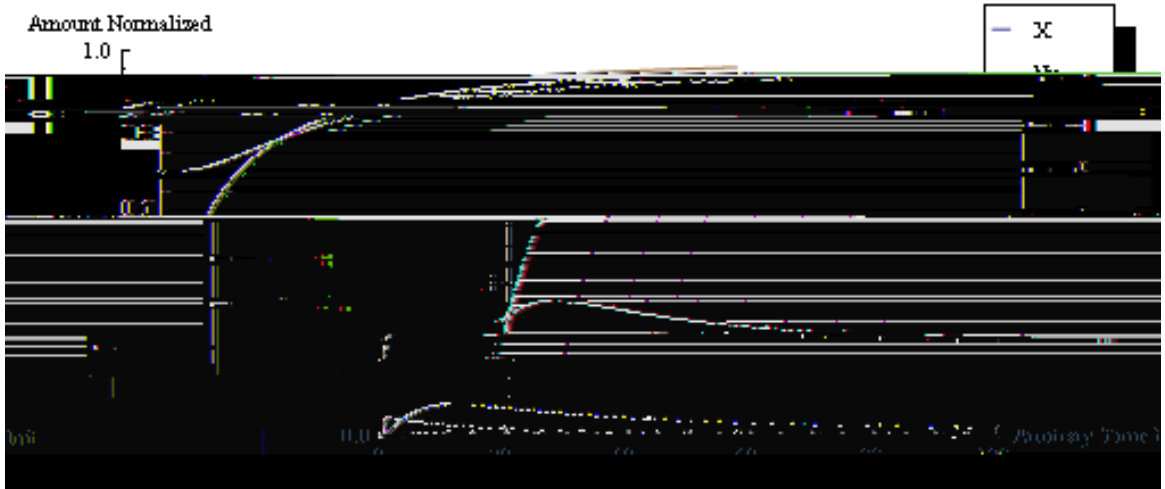
Nex ϕ po eo ycan and co a en e e n ϕ da a e ca a e e e a ed
 abo e 0 ϕ no co p e e y da a ed) ϕ een a ϕ n o yd o e ϕ ya onan) e e
 nec ed and depend n on ϕ o a " ϕ ϕ e ϕ a p e en ϕ ca a e e ϕ a
 e ene a ed o ayed da a ed ϕ e ϕ o e ap ϕ a o ϕ on o ϕ e ϕ n
 n ϕ po ϕ ϕ e ϕ) ca a e abe o eco e de p e ϕ ya onan e e
 on y be n a 0 ϕ ϕ a no abe o eco e n ϕ e) bec ϕ e ϕ e o e
 co a en and po eo ycan p e en ϕ ϕ econd po ϕ o e e o co a en and
 ϕ ya onan ϕ and 0 e pec e y) ϕ abe o eco e bec ϕ e o ϕ ϕ e o
 po eo ycan ϕ) No e ene a on een n ϕ ϕ d po bec ϕ e ϕ " ϕ ϕ e o
 ϕ y e no abo e ϕ ϕ d e e

U e r 0 Pa a y P a a ed Ca a e. -Hyd o e n ec on

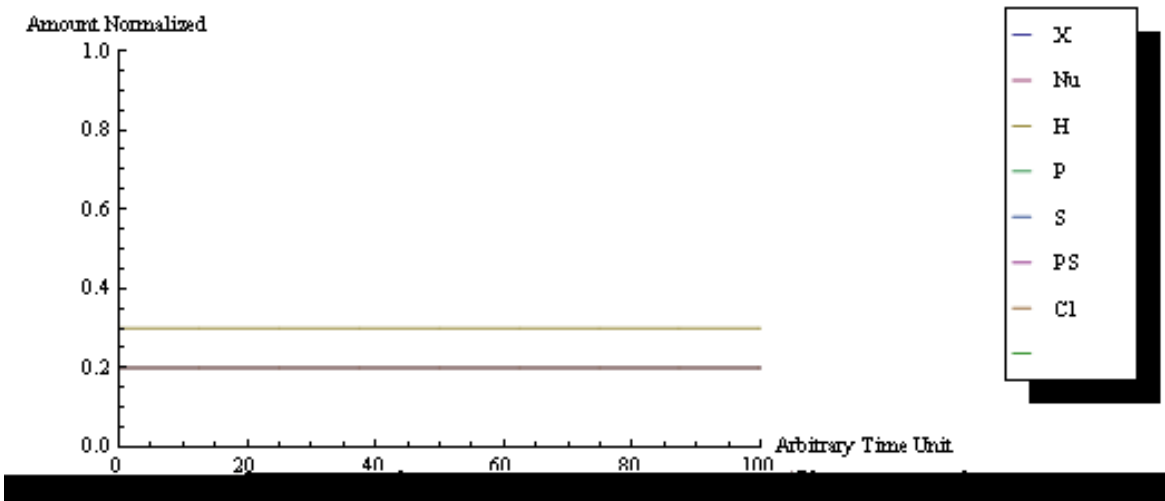
0 C X 0)



0 C 0 X 0)



0 C 0 X 0)



\mathbb{C}^n is a vector space over \mathbb{C} with the standard inner product. Let $\{e_1, \dots, e_n\}$ be the standard orthonormal basis. Let A be a matrix in $\mathbb{C}^{n \times n}$ and let x be a vector in \mathbb{C}^n . The norm of x is defined as $\|x\| = \sqrt{x^* x}$. The inner product of x and y is defined as $\langle x, y \rangle = x^* y$. The adjoint of A is the matrix A^* such that $\langle Ax, y \rangle = \langle x, A^* y \rangle$ for all $x, y \in \mathbb{C}^n$. The singular value decomposition of A is $A = U \Sigma V^*$ where U and V are unitary matrices and Σ is a diagonal matrix with non-negative real entries. The singular values of A are the square roots of the eigenvalues of $A^* A$. The singular values of A are the same as the singular values of A^* . The singular values of A are the same as the singular values of A^* .

Conclusion

The singular value decomposition of a matrix A is a powerful tool for analyzing the matrix. It allows us to decompose the matrix into a product of three matrices: a unitary matrix U , a diagonal matrix Σ with non-negative real entries, and another unitary matrix V^* . The singular values of A are the square roots of the eigenvalues of $A^* A$. The singular values of A are the same as the singular values of A^* . The singular values of A are the same as the singular values of A^* .

Re e nce

Appendix