Εργαστήριο Φυσικοχημείας

Διατριβές 2006-2010

Α. Διπλωματικές Εργασίες (Διατριβές Ειδικεύσεως) Master Theses

1. Β. Νουσίου
Υπολογιστική Μελέτη Ταλαντώσεων κατά την Οξείδωση του CO σε Αναδιατασσόμενη Επιφάνεια του Καταλύτη Pt(100)
2006, Επιστημονική Υπεύθυνος: Α. Προβατά, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Α. Τσεκούρας

V. Nousiou
Computational study of surface recosntruction and oscillations during the CO oxidation on catalyst Pt(100)
2006, Scientific Advisor: A. Provata, NCSR Demokritos, Academic Advisor: A. Tsekouras

2. Κ. Ποταμίτης
Χρήση φυσικοχημικών μεθόδων στη μελέτη διαμορφωτικής ανάλυσης του αντιυπερτασικού φαρμάκου Valsartan και αλληλεπιδράσεών του με λιποειδείς διπλοστοιβάδες
2006, Επιβλέπων: Κ. Βύρας

K. Potamitis
Use of physicochemical methods to investigate the conformational properties of the antihypertensive drug Valsartan and its interactions with membrane bilayers
2006, Advisor: K. Viras

3. Ε. Χαλκεύς
Διαμορφωτική ανάλυση του καινοτόμου φαρμακευτικού μορίου MMK2 με φυσικοχημικές μεθόδους και μελέτη των αλληλεπιδράσεών του με τις λιποειδείς διπλοστοιβάδες
2006, Επιβλέπων: Κ. Βύρας

I. Halkefs
Conformational analysis of the novel pharmaceutical molecule MMK2 using physicochemical methods and study its interactions with lipid bilayers
2006, Advisor: K. Viras

4. Α. Θανάσουλας
Μελέτη της θερμικής αποδιάταξης σε διάλυμα του πρωτεϊνικού μορίου HU του θερμόφιλου αρχαίου Thermoplasma volcanium με την τεχνική της αδιαβατικής μικροθερμοδομετρίας διαφορικής σάρωσης
2006, Επιστημονικός Υπεύθυνος: Γ. Νούνεσης, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Α. Τσεκούρας

A. Thanassoulas

Study of the thermal denaturation of the HU protein from the thermophilic Archaeon Thermoplasma volcanium by differential scanning microcalorimetry
2006, Scientific Advisor: G. Nounesis, NCSR Demokritos, Academic Advisor: A. Tsekouras

5. Ε. Μηλιόρδος
Θεωρητική μελέτη της ηλεκτρονιακής δομής των οξειδίων του βαναδίου, $VO^{0,\pm}$
2006, Επιβλέπων: Α. Μαυρίδης

E. Miliordos
Theoretical study of the electronic structure of vanadium oxides, $VO^{0,\pm}$
2006, Advisor: A. Mavridis

6. Μ. Τριμιθιώτου
Στατιστική μηχανική μελέτη ιοντικού διαλύματος Cl^-, Na^+/μεθανόλης σε υποκρίσιμη και υπερκρίσιμη κατάσταση μέσω μοριακής δυναμικής προσομοίωσης
2006, Επιβλέπων: Ι. Σάμιος

M. Trimithiotou
Statistical mechanics study of Cl^-, Na^+/methanol solution under subcritical and supercritical conditions via molecular dynamics simulation
2006, Advisor: J. Samios

7. Ν. Μαργέτης
Διαμοριακό δυναμικό και φαινόμενα μεταφοράς O_2^+ σε μερικώς πυκνό Kr υπό την επίδραση ηλεκτρικού πεδίου
2006, Επιβλέπων: Α. Κούτσελος

N. Margetis
Intermoolecular potential and transport phenomena of O_2^+ in partially dense Kr under the influence of an electric field
2006, Advisor: A. Koutselos

8. Ν. Ελπιδοφόρου
Στατιστική μηχανική μελέτη των ιδιοτήτων του υγρού μίγματος των οργανικών διαλυτών Ν,Ν-διμεθυλο-φορμαμιδίου (DMF) και Ν-μεθυλο-φορμαμιδίου (NMF)
2007, Επιβλέπων: Ι. Σάμιος

N. Elpidoforou
Statistical mechanics study of the properties of the liquid mixture of the organic solvents N,N-dimethylformamide (DMF) and N-methylformamide (NMF)
2007, Advisor: J. Samios

9. Π. Κακάτσου
Ανάπτυξη οξειδοαναγωγικών πολυμερικών ηλεκτρολυτών και εφαρμογή τους

σε ευαισθητοποιημένες ηλιακές κυψελίδες
2007, Επιστημονικός Υπεύθυνος: Π. Φαλάρας, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Κ. Βύρας

P. Kakatsou
Nano-composite polymer redox electrolytes for dye sensitized solar cells
2007, Scientific Advisor: P. Falaras, NCSR Demokritos, Academic Advisor: K. Viras

10. Π. Χατζηγεωργίου
Φυσικοχημική ανάλυση των αλλαγών φάσεως που παρουσιάζει το ρακεμικό μείγμα του φυσικού αμινοξέος DL-Norvaline και μελέτη της αλληλεπίδρασής του με μοντέλα βιολογικών μεμβρανών της DPPC
2007, Επιβλέπων: Κ. Βύρας

P. Chatzigeorgiou
Physicochemical analysis of phase transitions which are presented in the racemic compound of natural amino acid DL-Norvaline and its interactions with models of biological membranes, such as DPPC.
2007, Advisor: K. Viras

11. Παπαματθαιάκης Δημήτριος
Μικυλλιακές ιδιότητες της επιφανειοδραστικής ουσίας δισ-(2-αιθυλεξυλ)σουλφοηλεκτρικού νατρίου σε διαλύτες νερού αμιδίου
2008, Επιβλέπουσα: Β. Χαβρεδάκη

D. Papamatthaiakis
Micellization properties of surface active agent sodium bis-(2-ethylhexyl)sulfosuccinate in aqueous amide solution
2008, Advisor: V. Havredaki

12. Η. Λίτινας
Θερμοδυναμικές ιδιότητες και αλληλεπιδράσεις αμφίφιλων μορίων σε υδατικά διαλύματα αμινοξέων
2008, Επιβλέπουσα: Β. Χαβρεδάκη

H. Litinas
Micellar thermodynamics properties and interactions of amphiphile molecules in aqueous amino acids solutions
2008, Advisor: V. Havredaki

13. Α. Φωτιάδου
Μελέτη της αλληλεπίδρασης μεταξύ θετικώς και αρνητικώς φορτισμένων κυκλοδεξτρινών σε πολικά διαλύματα με Φασματοσκοπία NMR και Θερμιδομετρία Ισόθερμης Τιτλοδότησης
2009, Επιστημονική Υπεύθυνος: Κ. Γιαννακοπούλου, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Α. Παπακονδύλης

E. Fotiadou
Study of the interaction of positively and negatively charged cyclodextrines in polar solutions with NMR spectroscopy and isothermal titration calorimetry

2009, Scientific Advisor: K. Giannakopoulos, NCSR Demokritos, Academic Advisor: A. Papakondylis

14. Ν. Παπακωνσταντόπουλος
Φυσικοχημική μελέτη των αλληλεπιδράσεων των αμινοξέων DL-Norleucine και DL-Methionine με μοντέλλα μεμβρανών της DPPC
2009, Επιβλέπων: Κ. Βύρας

N. Papakonstantopoulos
Physicochemical study of the interactions of the amino acids DL-Norleucine and DL-Methionine with models of biological membranes such as DPPC
2009, Advisor: K. Viras

15. Δ. Χαρίση
Στατιστική μηχανική μελέτη της αγγειοτενσίνης ΙΙ σε διάλυμα νερού και νερού/αιθανόλης (65%:35%) για διάφορες θερμοκρασίες
2010, Επιβλέπων: Ι. Σάμιος

D. Charisi
Statistical mechanical study of angiotensin II in pure H_2O and (H_2O / EtOH) 65/35 solvents at different temperatures
2010, Advisor: J. Samios

16. Κ. Τσαμπαλής
Στατιστική μηχανική μελέτη ισορροπίας υγρής-αερίου φάσεως των καθαρών συστατικών SF6 και Xe καθώς και των δυαδικών μιγμάτων τους μέσω μοριακών προσομοιώσεων MD
2010, Επιβλέπων: Ι. Σάμιος

K. Tsampalis
Statistical mechanical study of the vapor – liquid equilibrium of the pure components SF_6 and Xenon as well as their binary mixtures through Molecular Dynamics Simulations
2010, Advisor: J. Samios

17. Α. Μουρελάτου
Μελέτη της αλληλεπίδρασης του βιοδραστικού μορίου tilifoside και του ακετυλιωμένο παραγώγου του με πρότυπες βιολογικές μεμβράνες DPPC
2010, Επιβλέπων: Κ. Βύρας

A. Mourelatou
Study of interactions of the bioactine molecule tiliroside and the acetyl derivative of tiliroside with models of biological membrane DPPC
2010, Advisor: K. Viras

18. Γ. Κούζιλος
Μελέτη μηχανικών και φυσικοχημικών ιδιοτήτων επαναμορφοποιημένων δειγμάτων πολυαιθυλενίου
2010, Επιβλέπων: Κ. Βύρας

G. Kouzilos

Study of mechanical and physicochemical properties of reformed polyethylene samples
2010, Advisor: K. Viras

B. Διδακτορικές Διατριβές
Ph. D. Theses

1. Ι. Σκαρμούτσος
Θεωρητική – υπολογιστική μελέτη της επίδρασης θερμοδυναμικών παραμέτρων στη διαμόρφωση των μακροσκοπικών, δομικών και δυναμικών ιδιοτήτων μοριακών συστημάτων στην υπερκρίσιμη κατάσταση
2006, Επιβλέπων: Ι. Σάμιος

I. Skarmoutsos
Theoretical – computational study of the effect of thermodynamic paramaters in the establishment of macroscopic, structural and dynamic properties of molecular systems in the hypercritical state
2006, Advisor: J. Samios

2. Κ. Κούκουνας
Ab initio διερεύνησις της ηλεκτρονιακής δομής των διατομικών μεταλλο-φθοριδίων MF, M = Fe, Co, Ni, και Cu
2007, Επιβλέπων: Α. Μαυρίδης

C. Koukounas
Ab intio investigation of the electronic structure of the diatomic metal fluorides MF, M = Fe, Co, Ni, and Cu
2007, Advisor: A. Mavridis

3. Σ. Καρδαχάκης
Ab initio υπολογισμοί επί των MCl
2007, Επιβλέπων: Α. Μαυρίδης

S. Kardahakis
Ab intio calculations on MCl
2007, Advisor: A. Mavridis

4. Π. Γκιάστας
Μοριακές δομές των βακτηριακών Φερρεδοξινών PaFd και EcFd
2007, Επιστημονική Υπεύθυνος: Ε. Μαυρίδου, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Α. Μαυρίδης

P. Giastas
Molecular structures of bacterial ferredoxins PaFd and EcFd
2007, Scientific Advisor: I. Mavridis, NCSR Demokritos, Academic Advisor: A. Mavridis

5. Β. Χαραλαμπόπουλος
Διερεύνηση πολυιωδιούχων συμπλόκων α- και β-κυκολδεξτρίνης με

μεταλλικά ιόντα μέσω διηλεκτρικής και Raman φασματοσκοπίας
2008, Επιβλέπων: Ι. Παπαϊωάννου

V. Charalampopoulos
Investigation of the poyiodide inclusion complexes of α- and β-cyclodextrin with metal ions via dielectric and Raman spectroscopy
2008, Advisor: I. Papaioannou

6. Σ. Χατζηευθυμίου
Κρυσταλλογραφική μελέτη δομής βιολογικών μακρομορίων. Ι. Ανοσοσφαιρινικού τύπου περιοχές 9 έως 11 της μυοσφαιρίνης. ΙΙ. Σύμπλοκα εγκλεισμού κυκλοδεξτρινών
2008, Επιστημονική Υπεύθυνος: Ε. Μαυρίδου, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Α. Μαυρίδης

S. Chatziefthimiou
Crystallographic study of biological macromolecules. I. Myomesin immunoglobulin domains 9-11. II. Cyclodextrin inclusion complexes
2008, Scientific Advisor: I. Mavridis, NCSR Demokritos, Academic Advisor: A. Mavridis

7. Β. Νουσίου
Υπολογιστική μελέτη δημιουργίας χωροχρονικών ταλαντώσεων σε ετερογενείς καταλυτικές αντιδράσεις
2008, Επιστημονική Υπεύθυνος: Α. Προβατά, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Α. Τσεκούρας

V. Noussiou
Computational study of the emergence of oscillations in heterogeneous catalytic reactions
2008, Scientific Advisor: A. Provata, NCSR Demokritos, Academic Advisor: A. Tsekouras

8. Ζ. Μακροδημήτρη
Προσομοίωση Μοριακής Δυναμικής της Μικροσκοπικής Δομής και των Φυσικοχημικών Ιδιοτήτων Ελαστομερών Πολυμερών
2009, Επιβλέπων: Ι. Σάμιος

Z. Makrodimitri
Molecular Dynamics Simulation of Microscopic Structure and physicochemical properties of elastomeric polymers
2009, Advisor: J. Samios

9. Γ. Λιθοξόος
Στατιστική μηχανική μελέτη προσροφήσεως ρευστών μοριακών συστημάτων σε νανοπορώδη υλικά άνθρακα και πυριτίου μέσω υπολογιστικών τεχνικών μοριακών προσομοιώσεων
2009, Επιβλέπων: Ι. Σάμιος

G. Lithoxoos
Theoretical – computational investigation of the adsorption of molecular

fluids in carbon and silicon nanoporous materials
2009, Advisor: J. Samios

10. Α. Θανάσουλας
Μελέτη δομικών μεταβολών σε πρωτεϊνικά μόρια με τη χρήση της τεχνικής της αδιαβατικής θερμιδομετρίας διαφορικής σάρωσης: Θερμοδυναμική με βάση τη δομή σταθερότητα της λειτουργικής περιοχής BRCT των πρωτεϊνών BRCA1, BARD1 και 53BP1
2009, Επιστημονικός υπεύθυνος: Γ. Νούνεσης, ΕΚΕΦΕ Δημόκριτος, Επιβλέπων: Κ. Βύρας

A. Thanasoulas
Study of structural changes in protein by differential scanning calorimetry: Structure-based thermodynamic stability of the BRCT domain of BRCA1, BARD1 and 53BP1
2009, Scientific Advisor: G. Nounesis, NCSR Demokritos, Academic Advisor: K. Viras

11. Ε. Πολλάτος
Μορφολογία και δομή των νανο-πολυμερικών υλικών και η συμπεριφορά τους σε εφαρμογές ηλεκτρομαγνητικής θωράκισης
2009, Επιβλέπων: Κ. Βύρας

E. Pollatos
Morphology and structure of nano-polymeric materials and their behaviour in electromagnetic shielding applications
2009, Advisor: K. Viras

12. Α. Λαμπρόπουλος
Ανάπτυξη σύνθετων μεμβρανών νανοδομών άνθρακα και πυριτίου για τον διαχωρισμό μειγμάτων αερίων και μελέτη νανοδομών άνθρακα για την αποθήκευση υδρογόνου
2009, Επιστημονικός Υπεύθυνος: Ν. Κανελλόπουλος, ΕΚΕΦΕ Δημόκριτος, Επιβλέπουσα: Β. Χαβρεδάκη

A. Labropoulos
Development of nanostructured carbon and silicon composite membranes for separation of gas mixtures and study of carbon nanostructures for hydrogen storage
2009, Scientific Advisor: N. Kanellopoulos, NSCR Demokritos, Academic Advisor: V. Havredaki

13. Ε. Μηλιόρδος
Ηλεκτρονιακή δομή των οξειδίων $MO^{0,\pm}$, M = Sc, Ti, Cr, Mn, μέσω υπολογισμών πρώτων αρχών
2010, Επιβλέπων: Α. Μαυρίδης

E. Miliordos
Electronic structure of $MO^{0,\pm}$ oxides, M = Sc, Ti, Cr, Mn, through ab initio calculations
2010, Advisor: A. Mavridis

14. Ι. Καρτσωνάκης
Ηλεκτροχημική εναπόθεση πολυλειτουργικών αγώγιμων πολυμερών για αντιδιαβρωτική προστασία μετάλλων
2010, Επιστημονικός Υπεύθυνος: Γ. Κόρδας, ΕΚΕΦΕ «Δημόκριτος, Επιβλέπουσα: Μ. Ανδριανοπούλου-Παλαιολόγου

I. Kartsonakis
Electrochemical deposition of multifunctional conductive polymers for corrosion protection of metals
2010, Scientific Advisor: G. Kordas, NCSR Demokritos, Academic Advisor: M. Andrianopoulou-Palaiologou

Εργαστήριο Φυσικοχημείας

Δημοσιεύσεις 2006-2010

Γ. Ερευνητικές εργασίες
Research papers

1. Aqueous gels of triblock copolymers of ethylene oxide and 1,2-butylene oxide (type BEB) studied by rheometry
Antonis Kelarakis, Vasiliki Havredaki, Xue-Feng Yuan, Chiraphon Chaibundit, Colin Booth
Macromol. Chem. Physic. **207** 903-909 (2006)
[DOI: 10.1002/macp.200600028]

2. Mixed quantum-classical molecular dynamics simulation of vibrational relaxation of ions in an electrostatic field
Andreas D. Koutselos
J. Chem. Phys. **125**, 244304 (2006) (8 pages)
[DOI: 10.1063/1.2424457]

3. The interaction of the early 3d-transition metals Sc, Ti, V, and Cr with N_2. An ab initio study
S. Kardahakis, C. Koukounas and A. Mavridis
J. Chem. Phys. **124**, 104306 (2006) (13 pages)
[DOI: 10.1063/1.2174000]

4. Ab initio study of the electronic structure of manganese carbide, MnC.
A. Kalemos, T. H. Dunning, Jr., and A. Mavridis
J. Chem. Phys. **124**, 154308 (2006)
[DOI: 10.1063/1.2181972]
Letter to the American Journal of Physics. "1937 Nobel Prize"
A. Mavridis
Am. J. Phys. **74**, 353 (2006)
[DOI: 10.1119/1.2166374]

5. The electronic structure of cobalt carbide, CoC
D. Tzeli and A. Mavridis
J. Phys. Chem. A **110**, 8952-8962 (2006)
[DOI: 10.1021/jp062357g]

6. Structure and energetics of gaseous HZnCl
I. S. K. Kerkines, A. Mavridis and P. A. Karipidis
J. Phys. Chem. A **110**, 10899-10903 (2006)
[DOI: 10.1021/jp062801f]

7. Surface Tension of 4-Methyl-2-Pentanone / Ethyl benzoate Binary System in the Temperature Range from 278.15 K to 308.15 K
Nikos G. Tsierkezos and Ioanna E. Molinou
J. Sol. Chem. **35**, 279-296 (2006)
[DOI: 10.1007/s10953-006-9365-x]

8. Transport properties of 2:2 symmetrical electrolytes in (water + ethylene glycol) binary mixtures at T = 293.15 K
Nikos G. Tsierkezos and Ioanna E. Molinou
J. Chem. Thermodyn. **38**, 1422-1431 (2006)
[DOI: 10.1016/j.jct.2006.01.011]

9. Thermodynamic investigation of dimethyl sulfoxide binary mixtures at 293.15 and 313.15 K
Maria M. Palaiologou, George K. Arianas and Nikos G. Tsierkezos
J. Sol. Chem. **35**, 1551-1565 (2006)
[DOI: 10.1007/s10953-006-9082-5]

10. Dielectric and Raman spectroscopy of the heptaiodide complex (β-Cyclodextrin)$_2$·CsI_7·13H_2O
Vasileios G. Charalampopoulos, John C. Papaioannou and Haido S. Karayianni
Solid State Sci. **8**, 97-103 (2006)
[DOI: 10.1016/j.solidstatesciences.2005.10.010]

11. AC-conductivity and Raman spectra of polyiodide inclusion compounds (β-cyclodextrin)$_2$·KI_7·16H_2O and (β-cyclodextrin)$_2$·LiI_7·14H_2O during the dehydration process
John C. Papaioannou, Vasileios G. Charalampopoulos, Pantelis Xynogalas and Kyriakos Viras
J. Phys. Chem. Solids **67**, 1379-1386 (2006)
[DOI: 10.1016/j.jpcs.2006.01.109]

12. SiC Nanotubes: A Novel Material for Hydrogen Storage
Giannis Mpourmpakis and George E. Froudakis, George P. Lithoxoos and Jannis Samios
Nano Lett. **6**, 1581-1883 (2006)
[DOI: 10.1021/nl0603911]

13. Local intermolecular structure and dynamics in binary supercritical solutions. A molecular dynamics simulation study of methane in carbon dioxide
Ioannis Skarmoutsos and Jannis Samios
J. Mol. Liq. **125**, 181-186 (2006)
[DOI: 10.1016/j.molliq.2005.11.023]

14. Local Density Inhomogeneities and Dynamics in Supercritical Water: A Molecular Dynamics Simulation Approach
I. Skarmoutsos and J. Samios
J. Phys. Chem. B **110**, 21931-21937 (2006)
[DOI: 10.1021/jp060955p]

15. Effect of a bioactive curcumin derivative on DPPC membrane: A DSC and Raman spectroscopy study
Kostantinos Gardikis, Sophia Hatziantoniou, Kyriakos Viras and Costas Demetzos
Thermochim. Acta **447** 1-4 (2006)
[DOI: 10.1016/j.tca.2006.03.007]

16. A DSC and Raman spectroscopy study on the effect of PAMAM dendrimer on DPPC model lipid membranes

Konstantinos Gardikis, Sophia Hatziantoniou, Kyriakos Viras, Matthias Wagner and Costas Demetzos
Int. J. Pharm. **318** 118-123 (2006)
[DOI: 10.1016/j.ijpharm.2006.03.023]

17. A Theoretical Study of Calcium Monohydride, CaH: Low-Lying States and Their Permanent Electric Dipole Moments
I. S. K. Kerkines and A. Mavridis
J. Phys. Chem. A **111**, 371-374 (2007)
[DOI: 10.1021/jp064705k]

18. The Electronic Structure of Vanadium Oxide. Neutral and Charged Species, $VO^{0,+-}$
E. Miliordos and A. Mavridis
J. Phys. Chem. A **111**, 1953-1965 (2007)
[DOI: 10.1021/jp067451b]

19. Theoretical investigation of the ground and low-lying excited states of Nickel Carbide, NiC
D. Tzeli and A. Mavridis
J. Chem. Phys. **126**, 194304 (2007) (12 pages)
[DOI: 10.1063/1.2723114]

20. All Electron First Principles Calculations of the Ground and Some Low-Lying Excited States of BaI
E. Miliordos, A. Papakondylis, A. A. Tsekouras, and A. Mavridis
J. Phys. Chem. A **111**, 10002-10009 (2007)
[DOI: 10.1021/jp0745788]

21. Ab initio Study of the Electronic Structure and Bonding of Aluminum Nitride, AlN
A. Kalemos and A. Mavridis
J. Phys. Chem. A **111**, 11221-11231 (2007) [invited paper, special issue dedicated to T. H. Dunning, Jr.]
[DOI: 10.1021/jp070544o]

22. Conductivity Studies of n-Tetrabutylammonium Tetraphenylborate in 3-Pentanone in the Temperature Range from 283.15 to 329.15 K
Nikos G. Tsierkezos and Ioanna E. Molinou
J. Sol. Chem. **36**, 153-170 (2007)
[DOI: 10.1007/s10953-006-9103-4]

23. Thermodynamic investigation of methyl salicylate/1-pentanol binary system in the temperature range from 278.15 K to 303.15 K
Nikos G. Tsierkezos and Ioanna E. Molinou
J. Chem. Thermodyn. **39**, 1110-1117 (2007)
[DOI: 10.1016/j.jct.2007.01.008]

24. A transformation $I_2 \cdot I^- \cdot I_2$ - $I_3^- \cdot I_2$ in the pentaiodide complex $(\alpha\text{-Cyclodextrin})_2 \cdot Cd_{0.5} \cdot I_5 \cdot 26H_2O$, detected via dielectric and Raman spectroscopy
Vasileios G. Charalampopoulos, John C. Papaioannou, and Konstantinos E. Tampouris

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