

# Владимир Иванович Пупышев



(06.08.1949 -16.06.2020)

Кроме квантовой химии как основного профессионального занятия, с именем Владимира Ивановича Пупышева связано на химфаке МГУ много всякого, очень креативного. Он рано начал преподавать, был любим студентами разных поколений, и сыграл колоссальную роль в развитии лучшего, что было на химфаке – «одиннадцатых групп». Это такая своего рода местная физматшкола, которая позволяет несколько ослабить груз классического химического образования, и в свободное от него время изучить довольно много полезных физмат-дисциплин. Благодаря 11 группе на химфак в трудные годы приходили выпускники сильных физматшкол, что конечно очень способствовало созданию среды. И не было равных Володе Пупышеву по части поддержания этой среды в дееспособном и жизнерадостном состоянии. Учиться у него было интересно и приятно, и учебный процесс плавно сливался с вне-аудиторным общением, которое сохранялось потом надолго, и происходило всегда совершенно на равных.

Пупышевский кругозор был безграничен, и не только в части квантовой химии - был он любопытен до много, включая даже обычную химию. И формулировать умел как-то непринужденно. Поэтому очень здорово было вместе с ним участвовать в разных жюри молодежных конференций, где важны вопросы нестандартные и оживляющие дискуссию. Удивительно умел никого не обижать, но, в то же время, замечать и обезвреживать любую глупость – редкий дар. И к конъюнктуре был совершенно равнодушен, премии и звания - если случайно перепали – довольно иронически воспринимал.

Еще «Советский химик», в давние времена – замечательная стенгазета, в которой наряду с идеологически выверенным содержанием выживали разные неформальные течения. Вспоминается в связи с Пупышевым чудесный персонаж, от имени которого иногда появлялись в этой газете всякие сообщения – звали персонажа Николай Нога, и был он чем-то вроде Евгения Сазонова в советской «Литературке». Под псевдонимом Н. Ноги скрывалось несколько авторов, и наблюдения за процессом их коллективного творчества были крайне увлекательны.

Верно коллеги сформулировали <http://www.chem.msu.ru/rus/Pupishev/welcome.html> - «исключительно талантливый ученый с ярким мышлением и безграничной эрудицией, человек невероятной доброты и бесконечной душевной щедрости». И пользовались мы все этой щедростью тоже бесконечно. А Володя в последние годы много и тяжело болел, но появлялся всегда на факультете как обычно, излучая оптимизм и интересуясь всем происходящим. Здесь <https://qpd.chem.msu.ru/memorial/> успели что-то о нем написать куда меньше людей, чем могли бы.

ГЦ

## Мемориальный доклад

Фрейдзон А.Я. «Памяти Владимира Ивановича Пупышева посвящается»  
[https://www.youtube.com/watch?v=a7IJ\\_yHyENk](https://www.youtube.com/watch?v=a7IJ_yHyENk)

## Учебники

1. Г.А. ЩЕМБЕЛОВ, Ю.А. УСТЫНЮК, В.М. МАМАЕВ, С.Я. ИЩЕНКО, И.П. ГЛОРИОЗОВ, В.Б. ЛУЖКОВ, В.В. ОРЛОВ, В.Я. СИМКИН, В.И. ПУПЫШЕВ, В.Н. БУРМИСТРОВ, КВАНТОВОХИМИЧЕСКИЕ МЕТОДЫ РАСЧЕТА МОЛЕКУЛ (РЕД. Ю.А. УСТЫНЮК). М., ХИМИЯ, 1980.
2. Н.Ф. СТЕПАНОВ, В.И. ПУПЫШЕВ, КВАНТОВАЯ МЕХАНИКА МОЛЕКУЛ И КВАНТОВАЯ ХИМИЯ, М.: ИЗД-ВО МГУ, 1991.
3. В.И. ПУПЫШЕВ, ДОПОЛНИТЕЛЬНЫЕ ГЛАВЫ КВАНТОВОЙ МЕХАНИКИ МОЛЕКУЛ. ВВЕДЕНИЕ В ТЕОРИЮ ССП. (ЧАСТИ1-3). М.: МГУ, 2008.

## Избранные статьи

1. CHANG, XH; KRASNOSHCHIEKOV, SV; PUPYSHEV, VI; MILLIONSHCHIKOV, DV.  
NORMAL ORDERING OF THE SU(1,1) LADDER OPERATORS FOR THE QUASI-NUMBER STATES OF THE MORSE OSCILLATOR  
PHYSICS LETTERS A 384(19), - (2020)
2. MONTGOMERY, HE; PUPYSHEV, VI.  
DIPOLE POLARIZABILITY FOR CONFINED TWO-ELECTRON ATOMIC SYSTEMS: SIMPLE APPROXIMATIONS  
PHYSICA SCRIPTA 95(1), - (2020)
3. PAZYUK, EA; PUPYSHEV, VI; ZAITSEVSKII, AV; STOLYAROV, AV.  
SPECTROSCOPY OF DIATOMIC MOLECULES IN AN ADIABATIC APPROXIMATION  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY A 93(10), 1865-1872 (2019)
4. PUPYSHEV, VI; MONTGOMERY, HE.  
ON THE SHELL-CONFINED ATOM PROBLEM  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 119(10), - (2019)
5. PUPYSHEV, VI; MONTGOMERY, HE.  
MONOTONICITY IN CONFINED SYSTEM PROBLEMS  
JOURNAL OF MATHEMATICAL CHEMISTRY 56(2), 493-507 (2018)
6. PUPYSHEV, VI; MONTGOMERY, HE.  
ONE- AND MULTICONFIGURATIONAL STUDY OF EXCITED STATES OF HE ATOM IN A SMALL IMPENETRABLE CAVITY

THEORETICAL CHEMISTRY ACCOUNTS 136(12), - (2017)

7. MONTGOMERY, HE; PUPYSHEV, VI.

FREQUENCY-DEPENDENT POLARIZABILITIES AND SHIELDING FACTORS FOR CONFINED ONE-ELECTRON SYSTEMS

PHYSICA SCRIPTA 92(1), - (2017)

8. BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.

TWO-DIMENSIONAL CHARACTER OF INTERNAL ROTATION OF FURFURAL AND OTHER FIVE-MEMBER HETEROCYCLIC AROMATIC ALDEHYDES

SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY 161, 155-161 (2016)

9. PUPYSHEV, VI; MONTGOMERY, HE.

SOME PROBLEMS IN APPLICATIONS OF THE LINEAR VARIATIONAL METHOD

EUROPEAN JOURNAL OF PHYSICS 36(5), - (2015)

10. PUPYSHEV, VI; MONTGOMERY, HE.

SPHERICALLY SYMMETRIC STATES OF HOOKIUM IN A CAVITY

PHYSICA SCRIPTA 90(8), - (2015)

11. MONTGOMERY, HE; PUPYSHEV, VI.

CONFINED TWO-ELECTRON SYSTEMS: EXCITED SINGLET AND TRIPLET S STATES

THEORETICAL CHEMISTRY ACCOUNTS 134(1), - (2014)

12. GODUNOV, IA; BATAEV, VA; ABRAMENKOV, AV; PUPYSHEV, VI.

THE BARRIERS TO INTERNAL ROTATION OF BENZALDEHYDE AND BENZOYL FLUORIDE: "RECONCILIATION" BETWEEN THEORY AND EXPERIMENT

JOURNAL OF PHYSICAL CHEMISTRY A 118(44), 10159-10165 (2014)

13. PUPYSHEV, VI; STEPANOV, NF.

SPECTROSCOPIC CHARACTERISTICS OF SIMPLE SYSTEMS IN A SPHERICAL CAVITY

RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY A 88(11), 1882-1888 (2014)

14. MONTGOMERY, HE; PUPYSHEV, VI.

CONFINED HELIUM: EXCITED SINGLET AND TRIPLET STATES

PHYSICS LETTERS A 377(40), 2880-2883 (2013)

15. MONTGOMERY, HE; PUPYSHEV, VI.

ON LOWER BOUNDS FOR POLARISABILITY

EUROPEAN PHYSICAL JOURNAL H 38(4), 519-534 (2013)

16. PUPYSHEV, VI; MONTGOMERY, HE.

HOW TO SPOIL A GOOD BASIS SET FOR RAYLEIGH-RITZ CALCULATIONS

JOURNAL OF MATHEMATICAL PHYSICS 54(8), - (2013)

17. PUPYSHEV, VI.

ELECTRONIC STATES OF HYDROGEN ATOM IN TETRAHEDRAL AND SIMILAR POLYHEDRAL CAVITIES

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 111(11), 2510-2518 (2011)

18. PUPYSHEV, VI.

NIKOLAI F. STEPANOV: HALF-A-CENTURY PASSION FOR QUANTUM CHEMISTRY

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 111(11), 2719-2725 (2011)

19. RASTOLTSEVA, EV; BATAEV, VA; ABRAMENKOV, AV; PUPYSHEV, VI; GODUNOV, IA.

STRUCTURE AND CONFORMATIONAL DYNAMICS OF THE DICYCLOPROPYL KETONE IN THE GROUND ELECTRONIC STATE

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 939(1-3), 14-21 (2010)

20. PUPYSHEV, VI; PAZYUK, EA; STOLYAROV, AV; TAMANIS, M; FERBER, R.  
ANALOGUE OF OSCILLATION THEOREM FOR NONADIABATIC DIATOMIC STATES: APPLICATION TO THE  
A(1)SIGMA(+) AND B(3)PI STATES OF KCS  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS 12(18), 4809-4812 (2010)
21. KRETOV, MK; SCHERBININ, AV; PUPYSHEV, VI.  
STATES OF A HYDROGEN ATOM IN AN IMPENETRABLE CUBIC CAVITY  
PHYSICA SCRIPTA 80(4), - (2009)
22. BOKAREVA, OS; BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.  
STRUCTURE AND DYNAMICS OF ACROLEIN IN (1,3)(PI,PI\*) EXCITED ELECTRONIC STATES: A QUANTUM-  
CHEMICAL STUDY  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY 73(4), 654-662 (2009)
23. BOKAREV, SI; PUPYSHEV, VI; GODUNOV, IA.  
VIBRONIC SPECTRA, AB INITIO CALCULATIONS, AND STRUCTURES OF CONFORMATIONALLY NON-RIGID  
MOLECULES OF OXALYL HALIDES IN THE GROUND AND LOWEST EXCITED ELECTRONIC STATES. PART II:  
THEORETICAL INVESTIGATION OF OXALYL CHLORIDE  
JOURNAL OF MOLECULAR SPECTROSCOPY 256(2), 247-255 (2009)
24. SEN, KD; PUPYSHEV, VI; MONTGOMERY, HE.  
EXACT RELATIONS FOR CONFINED ONE-ELECTRON SYSTEMS  
ADVANCES IN QUANTUM CHEMISTRY, VOL 57: THEORY OF CONFINED QUANTUM SYSTEMS: PT 1 57, 25-77  
(2009)
25. YURENEV, PV; SCHERBININ, AV; PUPYSHEV, VI.  
SHIFTS OF THE HYDROGEN ATOM IN A CYLINDRICAL CAVITY  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 108(14), 2666-2677 (2008)
26. BOKAREVA, OS; BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.  
STRUCTURE AND DYNAMICS OF ACROLEIN IN LOWEST EXCITED (1,3)(N,PI\*) ELECTRONIC STATES: THE  
QUANTUM-CHEMICAL STUDY  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 108(14), 2719-2731 (2008)
27. PANCHENKO, YN; DE MARE, GR; PUPYSHEV, VI; ABRAMENKOV, AV.  
VIBRATIONAL SPECTRA AND AB INITIO ANALYSIS OF TERT-BUTYL, TRIMETHYLSILYL, TRIMETHYLGERMYL,  
TRIMETHYLSTANNYL, AND TRIMETHYLPLUMBYL DERIVATIVES OF 3,3-DIMETHYLCYCLOPROPENE X. SOME  
REGULARITIES  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY 68(5), 1334-1339  
(2007)
28. BATAEV, V; KUDICH, A; ABRAMENKOV, A; PUPYSHEV, V; GODUNOV, I.  
THEORETICAL STUDY OF THE STRUCTURE OF 2-METHYLPROPANAL IN THE GROUND ELECTRONIC STATE:  
THREE-DIMENSIONAL MODEL FOR TORSIONAL VIBRATIONS  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 822(1-3), 133-144 (2007)
29. PUPYSHEV, VI.  
SIMPLEST PROOF OF THE JAHN-TELLER THEOREM FOR MOLECULAR SYSTEMS  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 107(6), 1446-1453 (2007)
30. YURENEV, PV; SCHERBININ, AV; PUPYSHEV, VI.  
ENERGY LEVELS OF THE HYDROGEN ATOM IN A CYLINDRICAL CAVITY  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 106(10), 2201-2207 (2006)
31. BOBRIKOV, VV; PUPYSHEV, VI.  
A DIATOMIC MOLECULE IN A SPHERICAL CAVITY

RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 79(9), 1472-1477 (2005)

32. PUPYSHEV, VI.

JAHN-TELLER THEOREM AND NODA POINTS OF WAVE FUNCTIONS

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 104(2), 157-166 (2005)

33. DOLGOV, EK; BATAEV, VA; PUPYSHEV, VI; ABRAMENKOV, AV; GODUNOV, IA.

ONE-DIMENSIONAL MODELS OF INTERNAL ROTATION IN CX<sub>3</sub>NO MOLECULES (X = H, D, F)

JOURNAL OF MOLECULAR SPECTROSCOPY 230(1), 43-53 (2005)

34. BOBRIKOV, VV; PUPYSHEV, VI.

ISOTOPE EFFECTS FOR MOLECULES IN A CAVITY

RUSSIAN CHEMICAL BULLETIN 54(1), 55-61 (2005)

35. DOLGOV, EK; BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.

STRUCTURE AND VIBRATIONS OF THE CF<sub>3</sub>NO MOLECULE IN THE GROUND AND LOWEST EXCITED ELECTRONIC STATES: A TEST OF AB INITIO METHODS

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 100(4), 509-518 (2004)

36. PUPYSHEV, VI; BOBRIKOV, VV.

THE CONFINED DIATOMIC MOLECULE PROBLEM

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 100(4), 528-538 (2004)

37. DOLGOV, EK; DOLGOVA, IV; BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.

A STUDY OF THE STRUCTURE OF THE CH<sub>3</sub>NO MOLECULE IN THE LOWER ELECTRONIC STATES BY MULTICONFIGURATION AB INITIO METHODS

RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 78(7), 1052-1058 (2004)

38. DOLGOV, EK; BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.

AB INITIO DESCRIPTION OF THE STRUCTURE AND DYNAMICS OF THE NITROSOMETHANE MOLECULE IN THE FIRST EXCITED SINGLET AND TRIPLET ELECTRONIC STATES

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 96(6), 589-597 (2004)

39. PUPYSHEV, VI; ERMILOV, AY.

BOUND STATES OF MULTIPOLES

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 96(3), 185-192 (2004)

40. CHANGA, ME; SCHERBININ, AV; PUPYSHEV, VI.

SPECTRA OF ONE-ELECTRON ATOM IN A SPHERICAL CAVITY

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 96(2), 167-174 (2004)

41. KUDICH, AV; BATAEV, VA; ABRAMENKOV, A; PUPYSHEV, VI; GODUNOV, IA.

THEORETICAL STUDY OF THE STRUCTURE OF PROPANAL IN THE FIRST EXCITED SINGLET AND TRIPLET ELECTRONIC STATES: THREE-DIMENSIONAL MODEL FOR TORSIONAL AND INVERSION VIBRATIONS

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 631, 39-51 (2003)

42. GODUNOV, IA; BATAEV, VA; YAKOVLEV, NN; PUPYSHEV, VI.

THE STRUCTURE OF CONFORMATIONALLY NONRIGID MOLECULES OF CARBONYL COMPOUNDS IN THE GROUND AND EXCITED ELECTRONIC STATES: EXPERIMENT AND THEORY

RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 76(11), 1732-1743 (2002)

43. PUPYSHEV, VI; SCHERBININ, AV.

HIDDEN SYMMETRY IN THE CONFINED HYDROGEN ATOM PROBLEM

PHYSICS LETTERS A 299(4), 371-376 (2002)

44. PUPYSHEV, VI.

HELLMANN-FEYNMAN THEOREM NEAR THE THRESHOLD

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 88(4), 380-391 (2002)

45. BATAEV, VA; DOLGOV, EK; ABRAMENKOV, AV; PUPYSHEV, VI; GODUNOV, IA.  
FEATURES OF THE FLUORINE-SUBSTITUTED ACETALDEHYDES DYNAMICS IN THE LOW-LYING ELECTRONIC STATES: QUANTUM MECHANICAL STUDY OF THE CHF<sub>2</sub>CHO MOLECULE LOWEST EXCITED SINGLET STATE  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 88(4), 414-425 (2002)

46. PAZYUK, EA; PUPYSHEV, VI; STOLYAROV, AV; KIYOSHIMA, T.  
MOLECULAR HYDROGEN 3S,D (3)LAMBDA(+)(G) COMPLEX REVISITED  
JOURNAL OF CHEMICAL PHYSICS 116(15), 6618-6627 (2002)

47. BATAEV, VA; MIKHAILOV, MN; ABRAMENKOV, AV; PUPYSHEV, VI; GODUNOV, IA.  
MOLECULAR STRUCTURE OF CHLORAL (CCL<sub>3</sub>CHO) IN THE LOWEST EXCITED SINGLET STATE  
JOURNAL OF STRUCTURAL CHEMISTRY 42(5), 723-729 (2001)

48. PAZYUK, EA; STOLYAROV, AV; PUPYSHEV, VI; STEPANOV, NF; UMANSKII, SY; BUCHACHENKO, AA.  
THE I-2(B) PREDISSOCIATION BY SOLVING AN INVERSE ATOMS-IN-MOLECULE PROBLEM  
MOLECULAR PHYSICS 99(2), 91-101 (2001)

49. BATAEV, VA; MIKHAILOV, MN; ABRAMENKOV, AV; PUPYSHEV, VI; GODUNOV, IA.  
MOLECULAR STRUCTURE AND CONFORMATIONS OF CHLORAL (CCL<sub>3</sub>CHO) IN THE GROUND AND LOWEST TRIPLET STATES  
JOURNAL OF STRUCTURAL CHEMISTRY 42(1), 57-65 (2001)

50. BATAEV, VA; PUPYSHEV, VI; ABRAMENKOV, AV; GODUNOV, IA.  
ONE- AND TWO-DIMENSIONAL MODELS OF TORSIONAL AND INVERSION VIBRATIONS IN 2-CHLOROETHANAL IN THE LOWEST TRIPLET EXCITED STATE  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 74(11), 1749-1757 (2000)

51. PANCHENKO, YN; PUPYSHEV, VI; BOCK, CW.  
VIBRATIONAL ANHARMONICITY AND SCALING THE QUANTUM MECHANICAL MOLECULAR FORCE FIELD  
JOURNAL OF MOLECULAR STRUCTURE 550, 495-504 (2000)

52. SCHERBININ, A; PUPYSHEV, VI.  
CHANGE OF IONIZATION PROPERTIES OF A MOLECULAR SYSTEM NEAR A SURFACE  
IZVESTIYA AKADEMII NAUK SERIYA FIZICHESKAYA 64(8), 1506-1510 (2000)

53. PUPYSHEV, VI.  
ON THE REPULSIVE NATURE OF THE DIRICHLET BOUNDARIES IN THE CONFINED ATOM PROBLEM  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 33(5), 961-970 (2000)

54. CHANGA, ME; SCHERBININ, AV; PUPYSHEV, VI.  
PERTURBATION THEORY FOR THE HYDROGEN ATOM IN A SPHERICAL CAVITY WITH OFF-CENTRE NUCLEUS  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 33(3), 421-432 (2000)

55. SHCHERBININ, AV; PUPYSHEV, VI.  
HYDROGEN ATOM IN A SPHERICAL CAVITY: DEGENERACY OF ENERGY LEVELS AND BOUNDARY CONDITIONS  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 74(2), 292-295 (2000)

56. PUPYSHEV, VI.  
WALL EFFECTS ON THE STATE OF A HYDROGEN ATOM IN A CAVITY  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 74(1), 50-54 (2000)

57. BATAEV, VA; PUPYSHEV, VI; ABRAMENKOV, AV; GODUNOV, IA.  
QUANTUM-MECHANICAL CALCULATIONS OF THE STRUCTURE AND DYNAMICS OF CONFORMATIONALLY NONRIGID CARBONYL COMPOUND MOLECULES IN THE GROUND AND EXCITED ELECTRONIC STATES  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 74, S279-S291 (2000)

58. PUPYSHEV, VI.  
THE NONTRIVIALITY OF THE HELLMANN-FEYNMAN THEOREM  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 74, S267-S278 (2000)
59. MIKHAILOVA, TY; PUPYSHEV, VI.  
EVOLUTION OF ONE-DIMENSIONAL QUANTUM SYSTEMS: TECHNIQUE FOR SEPARATION  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 74(1), 30-33 (2000)
60. PUPYSHEV, VI; SCHERBININ, AV.  
MOLECULAR ENERGY LEVEL SHIFTS IN LARGE BOXES: USE OF THE KIRKWOOD-BUCKINGHAM METHOD  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 32(19), 4627-4634 (1999)
61. BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.  
AB INITIO CALCULATIONS OF THE STRUCTURE AND DYNAMICS OF THE H<sub>2</sub>CO, F<sub>2</sub>CO, AND CL<sub>2</sub>CO  
MOLECULES IN ELECTRONICALLY EXCITED STATES  
RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY 73(9), 1448-1452 (1999)
62. MIKHAILOVA, TY; PUPYSHEV, VI.  
RESONANCES ON GRIDS  
OPTICS AND SPECTROSCOPY 87(1), 29-35 (1999)
63. MIKHAILOVA, TY; PUPYSHEV, VI.  
SYMMETRIC APPROXIMATIONS FOR THE EVOLUTION OPERATOR  
PHYSICS LETTERS A 257(1-2), 1-6 (1999)
64. BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.  
STRUCTURE AND DYNAMICS OF CONFORMATIONALLY NON-RIGID MOLECULES IN EXCITED ELECTRONIC  
STATES: AB INITIO CALCULATIONS OF THE R<sub>2</sub>CO (R = H, F, CL)  
JOURNAL OF MOLECULAR STRUCTURE 481, 263-267 (1999)
65. GODUNOV, IA; ABRAMENKOV, AV; BATAEV, VA; PUPYSHEV, VI.  
POTENTIAL FUNCTIONS OF INVERSION OF R<sub>2</sub>CO (R = H, F, CL) MOLECULES IN THE LOWEST EXCITED  
ELECTRONIC STATES  
RUSSIAN CHEMICAL BULLETIN 48(4), 640-646 (1999)
66. PUPYSHEV, V; SCHERBININ, AV.  
THE LENZ VECTOR IN THE CONFINED HYDROGEN ATOM PROBLEM  
CHEMICAL PHYSICS LETTERS 295(3), 217-222 (1998)
67. MIKHAILOVA, TY; PUPYSHEV, VI.  
ALGEBRAIC METHOD FOR THE EVOLUTION OPERATOR APPROXIMATION  
JOURNAL OF PHYSICS A-MATHEMATICAL AND GENERAL 31(18), 4263-4275 (1998)
68. BATAEV, VA; PUPYSHEV, VI; GODUNOV, IA.  
AB INITIO STUDY OF TORSIONAL VIBRATIONS OF THE FLUORAL MOLECULE IN THE GROUND STATE  
JOURNAL OF STRUCTURAL CHEMISTRY 39(3), 419-425 (1998)
69. PUPYSHEV, VI; SCHERBININ, AV; STEPANOV, NF.  
THE KIRKWOOD-BUCKINGHAM VARIATIONAL METHOD AND THE BOUNDARY VALUE PROBLEMS FOR THE  
MOLECULAR SCHRÖDINGER EQUATION  
JOURNAL OF MATHEMATICAL PHYSICS 38(11), 5626-5633 (1997)
70. SCHERBININ, AV; PUPYSHEV, VI; ERMILOV, AY.  
ONE-ELECTRON ATOM IN A CAVITY AS A MODEL FOR THE ELECTRONIC STRUCTURE OF INTERNAL ATOMS IN  
A CLUSTER  
IZVESTIYA AKADEMII NAUK SERIYA FIZICHESKAYA 61(9), 1779-1783 (1997)

71. ERMILOV, AY; PUPYSHEV, VI; STEPANOV, NF.  
CHANGES IN GEOMETRIC PARAMETERS OF BENZENE MOLECULE IN (C<sub>6</sub>H<sub>6</sub>)(N) ... LI-M SYSTEMS  
IZVESTIYA AKADEMII NAUK SERIYA FIZICHESKAYA 61(9), 1822-1826 (1997)
72. STOLYAROV, AV; PUPYSHEV, VI; CHILD, MS.  
ANALYTICAL APPROXIMATIONS FOR ADIABATIC AND NON-ADIABATIC MATRIX ELEMENTS OF  
HOMONUCLEAR DIATOMIC RYDBERG STATES. APPLICATION TO THE SINGLET P-COMPLEX OF THE  
HYDROGEN MOLECULE  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 30(14), 3077-3093 (1997)
73. PAZYUK, EA; STOLYAROV, AV; PUPYSHEV, VI.  
IMPROVEMENT ON VAN VLECK'S FORMULA FOR DIATOMIC NONADIABATIC ENERGY SHIFTS  
CHEMICAL PHYSICS LETTERS 267(3-4), 207-214 (1997)
74. GODUNOV, IA; ABRAMENKOV, AV; PUPYSHEV, VI.  
REINTERPRETATION OF THE FLUORESCENCE EXCITATION SPECTRUM OF HEXAFLUOROBIACETYL IN A  
SUPERSONIC JET  
JOURNAL OF STRUCTURAL CHEMISTRY 38(2), 236-243 (1997)
75. BUCHACHENKO, AA; MIKHAILOVA, TY; PUPYSHEV, VI; STEPANOV, NF.  
APPLICATION OF THE NON-HERMITEAN EFFECTIVE HAMILTONIAN METHOD TO METASTABLE VAN DER  
WAALS COMPLEXES  
12TH SYMPOSIUM AND SCHOOL ON HIGH-RESOLUTION MOLECULAR SPECTROSCOPY 3090, 57-61 (1997)
76. SCHERBININ, AV; PUPYSHEV, VI; STEPANOV, NF.  
ON THE USE OF MULTIPOLE EXPANSION OF THE COULOMB POTENTIAL IN QUANTUM CHEMISTRY  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 60(4), 843-852 (1996)
77. ERMILOV, AY; PUPYSHEV, VI; STEPANOV, NF.  
ELECTRON CORRELATION EFFECTS IN THE C<sub>6</sub>H<sub>6</sub>LI<sub>2</sub> SYSTEM  
ZHURNAL FIZICHESKOI KHIMII 70(11), 2019-2022 (1996)
78. PUPYSHEV, VV; SOLOVTSOVA, OP.  
ROLE OF THE INTERACTION BETWEEN NEUTRON MAGNETIC MOMENTS IN NEUTRON-NEUTRON  
SCATTERING  
PHYSICS OF ATOMIC NUCLEI 59(10), 1745-1754 (1996)
79. PANCHENKO, YN; DEMARE, GR; PUPYSHEV, VI.  
TESTING THE VALIDITY OF SCALING THE QUANTUM MECHANICAL MOLECULAR FORCE FIELDS FOR  
ROTATIONAL ISOMERS (VOL 99, PG 17548, 1995)  
JOURNAL OF PHYSICAL CHEMISTRY 100(26), 11202-11202 (1996)
80. ERMILOV, AY; FREIDZON, AY; PUPYSHEV, VI; STEPANOV, NF.  
MODELING THE ELECTRONIC STRUCTURE OF GRAPHITE INTERCALATION COMPOUNDS WITH LITHIUM BY  
METAL COMPLEXES WITH POLYBENZENE SYSTEMS  
JOURNAL OF STRUCTURAL CHEMISTRY 37(3), 392-397 (1996)
81. PUPYSHEV, VI; STEPANOV, NF; KRASNOSHCHIOKOV, SV; DEMARE, GR; PANCHENKO, YN.  
SOME ASPECTS OF SCALING THE MOLECULAR QUANTUM MECHANICAL FORCE FIELD  
JOURNAL OF MOLECULAR STRUCTURE 376, 363-368 (1996)
82. PANCHENKO, YN; DEMARE, GR; PUPYSHEV, VI.  
TESTING THE VALIDITY OF SCALING THE QUANTUM-MECHANICAL MOLECULAR-FORCE FIELDS FOR  
ROTATIONAL ISOMERS  
JOURNAL OF PHYSICAL CHEMISTRY 99(49), 17544-17550 (1995)



83. PAZYUK, EA; STOLYAROV, AV; PUPYSHEV, VI.  
APPROXIMATE SUM-RULE FOR DIATOMIC VIBRONIC STATES AS A TOOL FOR THE EVALUATION OF  
MOLECULAR-PROPERTIES  
CHEMICAL PHYSICS LETTERS 228(1-3), 219-224 (1994)
84. PUPYSHEV, VI; PANCHENKO, YN; STEPANOV, NF.  
A NEW DERIVATION FOR THE TELLER-REDLICH ISOTOPIC PRODUCT RULE  
VIBRATIONAL SPECTROSCOPY 7(2), 191-196 (1994)
85. STOLYAROV, AV; PUPYSHEV, VI.  
APPROXIMATE SUM-RULE FOR DIATOMIC VIBRONIC STATES  
PHYSICAL REVIEW A 49(3), 1693-1697 (1994)
86. KOZLOV, VA; PUPYSHEV, VI.  
SELF-CONSISTENT BRUECKNER THEORY FOR MOLECULAR-ORBITALS  
CHEMICAL PHYSICS LETTERS 206(1-4), 151-155 (1993)
87. ERMILOV, AY; KHRUSTOV, VF; PUPYSHEV, VI; STEPANOV, NF.  
MOLECULAR-MODELS OF COMPOUNDS OF LITHIUM INTERCALATION TO GRAPHITE  
ZHURNAL FIZICHESKOI KHIMII 67(1), 117-122 (1993)
88. PUPYSHEV, VI; PANCHENKO, YN; DEMARE, GR; BOCK, CW.  
SOME PROPERTIES OF REGULAR AND CANONICAL FORCE-FIELDS  
JOURNAL OF MOLECULAR STRUCTURE 272, 145-159 (1992)
89. PUPYSHEV, VI; MASTRYUKOV, VS.  
DEPENDENCE OF IONIZATION-POTENTIALS ON VALENT ANGLES IN HETEROCYCLIC-COMPOUNDS  
ZHURNAL FIZICHESKOI KHIMII 66(7), 1922-1926 (1992)
90. MIKHAILOV, TY; PUPYSHEV, VI.  
RELATIONSHIP BETWEEN ADIABATIC-APPROXIMATION ENERGY AND HARTREE-APPROXIMATION ENERGY IN  
THE PROBLEM ON COUPLED OSCILLATORS  
OPTIKA I SPEKTROSKOPIYA 72(2), 265-270 (1992)
91. GANELIN, PV; PUPYSHEV, VI.  
ANALYTIC PROPERTIES OF SOLUTION OF ELECTRONIC SCHRODINGER-EQUATION  
THEORETICAL AND MATHEMATICAL PHYSICS 88(1), 694-698 (1991)
92. PUPYSHEV, VI; PANCHENKO, YN; BOCK, CW; PONGOR, G.  
HARMONIC FORCE-FIELD - AN APPROXIMATE RELATIONSHIP BETWEEN THE EXACT NONRELATIVISTIC AND  
THE HARTREE-FOCK LIMIT VALUES OF THE FORCE-CONSTANTS  
JOURNAL OF CHEMICAL PHYSICS 94(2), 1247-1252 (1991)
93. BOCK, CW; PANCHENKO, YN; PUPYSHEV, VI.  
EFFECT OF BASIC SET QUALITY AND ELECTRON CORRELATION ON THE SCALE FACTORS OF A HARMONIC  
FORCE-FIELD  
JOURNAL OF COMPUTATIONAL CHEMISTRY 11(5), 623-628 (1990)
94. BOCK, CW; MCDIARMID, R; PANCHENKO, YN; PUPYSHEV, VI; KRASNOSHCHIOKOV, SV.  
TRANSFERABILITY OF QUANTUM-MECHANICAL FORCE-FIELD SCALE FACTORS BETWEEN CONJUGATED  
HYDROCARBONS  
JOURNAL OF MOLECULAR STRUCTURE 222(3-4), 415-429 (1990)
95. KOZLOV, VA; PUPYSHEV, VI; STEPANOV, NF.  
CALCULATION OF PROBABILITIES FOR BO-MOLECULE A<sub>2</sub>-PI-I-X<sub>2</sub>-SIGMA+ TRANSITION USING  
NONORTHOGONAL MOLECULAR-ORBITALS

OPTIKA I SPEKTROSKOPIYA 68(5), 1021-1024 (1990)

96. CHURAKOV, AV; MIKHAILOVA, TY; PAVLOVVEREVKIN, VB; PUPYSHEV, VI.  
N-LEVELS AND ONE CONTINUUM - BOUND-STATES IN CONTINUUM AND DEPENDENCE OF RESONANCE  
PARAMETERS ON THE COUPLING STRENGTH  
PHYSICS LETTERS A 144(2), 86-90 (1990)

97. KOZLOV, VA; PUPYSHEV, VI; STEPANOV, NF.  
THE EFFECT OF NONORTHOGONALITY OF ELECTRON WAVE-FUNCTIONS ON THE ESTIMATION OF THE  
TRANSITION DIPOLE-MOMENT  
TEORETICHESKAYA I EKSPERIMENTALNAYA KHIMIYA 26(2), 215-217 (1990)

98. PUPYSHEV, VI; KOZLOV, VA; KUZNETSOVA, LA.  
DISSOCIATIVE LIMIT OF DIPOLE-MOMENT OF DIATOMIC-MOLECULE TRANSITION  
OPTIKA I SPEKTROSKOPIYA 64(6), 1228-1233 (1988)

99. KUZMENKO, NE; PUPYSHEV, VI; STOLYAROV, AV.  
ON THE ESTIMATION OF EXCITED ELECTRON-STATE LIFETIME - APPLICATION TO A NAH MOLECULE  
OPTIKA I SPEKTROSKOPIYA 63(4), 756-761 (1987)

100. PUPYSHEV, VI.  
ON THE LIFETIME ESTIMATION FOR EXCITED ELECTRONIC STATE - THEORY  
OPTIKA I SPEKTROSKOPIYA 63(3), 570-574 (1987)

101. BOCK, CW; PANCHENKO, YN; KRASNOSHCHIOKOV, SV; PUPYSHEV, VI.  
AB INITIO STRUCTURES AND VIBRATIONAL ANALYSIS OF 2 PLANAR CONFIGURATIONS OF 1,3,5-HEXATRIENE  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 33(1-2), 131-140 (1986)

102. PUPYSHEV, VI; KRASNOSHCHIOKOV, SV; PANCHENKO, YN.  
FORCE-CONSTANTS AND MOLECULAR-POTENTIAL FUNCTIONS IN REDUNDANT COORDINATES  
JOURNAL OF MOLECULAR STRUCTURE 131(3-4), 347-356 (1985)

103. PANCHENKO, YN; PUPYSHEV, VI; ABRAMENKOV, AV; TRAETTEBERG, M; CYVIN, SJ.  
POTENTIAL FUNCTION OF INTERNAL-ROTATION FOR ISOPRENE FROM ABINITIO CALCULATIONS AND  
EXPERIMENTAL-DATA  
JOURNAL OF MOLECULAR STRUCTURE 130(3-4), 355-359 (1985)

104. BOCK, CW; PANCHENKO, YN; KRASNOSHCHIOKOV, SV; PUPYSHEV, VI.  
STRUCTURE AND VIBRATIONAL ASSIGNMENT OF GAUCHE-1,3-BUTADIENE  
JOURNAL OF MOLECULAR STRUCTURE 129(1-2), 57-67 (1985)

1059. SERGEEV, GB; STEPANOV, NF; LEENSON, IA; SMIRNOV, VV; PUPYSHEV, VI; TYURINA, LA;  
MASHYANOV, MN.  
MOLECULAR MECHANISM OF HYDROGEN BROMIDE ADDITION TO OLEFINS  
TETRAHEDRON 38(16), 2585-2589 (1982)

106. SIMKIN, VY; DEMENTEV, AI; PUPYSHEV, VI.  
POTENTIAL SURFACES OF BASIC AND EXCITED ELECTRON CONDITIONS OF CO<sub>2</sub> MOLECULES .1. A-1-  
1(SIGMA-1+G), B-1-2 AND B-3-2 CONDITIONS  
ZHURNAL FIZICHESKOI KHIMII 56(11), 2836-2838 (1982)

107. AROCA, R; ROBINSON, EA; PANCHENKO, YN; PUPYSHEV, VI.  
ON THE TORSIONAL INTERNAL COORDINATE IN MOLECULAR VIBRATIONS  
ACTA CHIMICA ACADEMIAE SCIENTARUM HUNGARICAE 110(4), 471-479 (1982)

108. MOSKOVSKAYA, TE; PUPYSHEV, VI; VITKOVSKAYA, NM.  
A PROGRAM FOR NON-EMPIRICAL CALCULATIONS FOR SYSTEMS WITH OPEN-SHELLS

JOURNAL OF STRUCTURAL CHEMISTRY 22(6), 930-931 (1981)

109. RAMBIDI, NG; STEPANOV, NF; ABASHKIN, YG; DEMENTEV, AI; ZHILINSKII, BI; MIKHALKO, VK; PUPYSHEV, VI; SIMKIN, VY; TOPOL, IA.

A THEORETICAL-STUDY OF THE MOLECULE OF BORIC OXIDE B<sub>2</sub>O<sub>3</sub>

JOURNAL OF STRUCTURAL CHEMISTRY 22(1), 21-28 (1981)

110. MAKHNIOV, AS; PUPYSHEV, VI; PANCHENKO, YN; STEPANOV, NF.

EXTREME VALUES OF MEAN-SQUARE AMPLITUDES OF MOLECULAR VIBRATIONS

JOURNAL OF MOLECULAR STRUCTURE 43(1), 101 (1978)

111. STEPANOV, NF; PUPYSHEV, VI.

ERRORS IN MOLECULAR INTEGRALS - INFLUENCE ON RHF ENERGY VALUES

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 11(1), 1 (1977)

112. AROCAM, R; ROBINSON, EA; PANCHENKO, YN; PUPYSHEV, VI.

ITERATIVE CONSISTENCY METHOD AND ITS GEOMETRIC INTERPRETATION

CHEMICAL PHYSICS LETTERS 43(2), 387 (1976)