Indian J. Phys. **76B** (**4**), 353–357 (2002)

I J P B
— an international journal

Above and below Wannier threshold ionization

D S F Crothers and N C Deb

Theoretical and Computational Physics Research Division, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

E-mail : d.crothers@qub.ac.uk

Abstract : The unifrom, semiclassical wave function of Crothers [*J. Phys.* **B19** 463 (1986)] for the two outgoing electrons has been analytically continued to below and then back above the threshold energy. For the case of below threshold ionization [*Phys. Rev. Lett.* **79** 4996 (1997), *J. Phys.* **B31** 2153 (1998)] we calculate complex eigenenergies for doubly excited states of He using a complex Bohr-Sommerfeld quantization rule with at least one complex transition point. The real parts of the eigenvalues give the resonance energy positions of He^{-*} found to be in good agreement with the measurement. The imaginary part leads to a good scaling of the intensities. In the case of above threshold ionization we achieve [*J. Phys.* **B33** L623 (2000), *J. Phys.* **B34** 143 (2001)] significant improvement in the triple differential cross sections for electron impact single ionization, over the previous calculations both in symmetric and asymmetric geometry with equal energy sharing by the two outgoing electrons. The results are compared with the latest measurements where ever available.

Keywords : Threshold ionization, resonance energy positions.

PACS Nos. : 31.15.–p, 31.50.+w, 34.80.Dp

Indian J. Phys. **76B** (**4**), 359–369 (2002)

I J P B
— an international journal

Quasi-atoms, super-atoms and quantum confinement

J-P Connerade
Department of Physics, Imperial College, London SW7 2BW, UK
E-mail : atomic_clusters@compuserve.com

Abstract : The terms ‘quasiatom’ and ‘superatom’ are introduced. A quasi-atom, for example contains two ions of opposite charge, which behave like an atom, forming Rydberg states. A superatom also contains many atoms, but behaves in a simple way, and can be modelled within the central field approximation. Both are examples of many-body systems which emulate quasi-particle properties. Their behaviour is the opposite of quasi-particle breakdown in isolated atoms. However, it also probes the boundary between simple and complex behaviour, for species larger than atoms. Examples are given, ranging from shallow donor impurities in semiconductors, through ion-pair molecules, confined and endohedral atoms, to metallic clusters.

Keywords : Endohedral atoms; clusters; semiconductors.

PACS No. : 36.10.–k

Indian J. Phys. **76B** (**4**), 371–378 (2002)

I J P B
— an international journal

New insights into small-angle electron scattering : guiding measurements

A Z Msezane and Z Felfli

Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA 30314, USA

E-mail : amsezane@ctsps.cau.edu

Abstract : Firstly, we demonstrate that in an appropriate representation the apparent generalized oscillator strength (AGOS) manifests its general properties and that the zero scattering angle curve connects continuously the threshold energy $E = w$ and the high energy $E = ¥$, corresponding to the optical oscillator strength, without traversing the nonphysical region. Secondly, the recent generalized Lassettre expansion (GLE) [*Phys. Rev. Lett.* **81** 961 (1998)] with only a single moving Regge pole is employed to establish the applicability of the Lassettre limit theorem regardless of the electron impact energy and to generate the associated normalization curve for the measured relative electron differential cross sections (DCS's). At forward scattering the GLE yields the unique and long-sought-after normalization curve to the optical oscillator strength of the measured relative DCS's through the AGOS. Optically allowed transitions in H, He and Xe are used to illustrate the normalization curve.

Keywords : Electron, scattering, oscillator, regge pole.

PACS Nos. : 34.80.Dp, 31.50.Df, 32.70.Cs, 34.10.+x

Indian J. Phys. **76B** (**4**), 379–385 (2002)

I J P B
— an international journal

Single and multiple ionization of atoms by electron impact

Hubert Klar
Theoretical Quaantumdynamics, Albert-Ludwige-Universität, Hermann Herder Strasse 3, 79104 Freiburg, Germany
E-mail : klarhub@RUF.UNI-FREIBURG.DE

Abstract : We report progress achieved during decades on direct single and multiple ionization of simple atoms by electron collsion. In particular we investigate total cross sections from threshold to high energies. We show that all experimental data compare favorably with Wannier threshold theory. A better understanding of the ionization process one gets from the analysis of multiply differential cross sections. To this end we discuss (e, 2e) and (e, 3e) events.

Keywords : Single, multiple, ionisation, electron, atom.

PACS No. : 34.80.Dp

Indian J. Phys. **76B** (**4**), 387–392 (2002)

I J P B
— an international journal

Laser cooling, evaporative cooling and Bose-Einstein condensation

Pradip N Ghosh
Department of Physics, University of Calcutta, 92, A.P.C. Road, Kolkata-700 009, India
E-mail : png@cubmb.ernet.in

Abstract : Laser radiations are used to slow down atoms by the process of momentum transfer. This leads to reducing the temperature to microkelvin region. Gas phase atoms are trapped by using magnetic fields. The recent advances have led to the realization of the dream of physicists of confining the atoms and reducing their velocities to the limit imposed by quantum mechanics. A number of new experiments are possible with the cooled and trapped atoms and ions that would be useful to solve many problems of theoretical physics. Further cooling by the process of evaporative technique has led to the observation of Bose-Einstein Condensation predicted by Einstein and Rose nearly seventy-five years ago. A brief review of the method of laser cooling, magnetic trapping and evaporative cooling methods used for obtaining ultracold atoms are discussed. It is possible to obtain temperature in the nanokelvin region without using cryogenic methods thus simplifying the experimental methods to a great extent.

Keywords : Laser, evaporative, cooling, B-E condensation.

PACS No. : 74.20.Fg

Indian J. Phys. **76B** (**4**), 393–400 (2002)

I J P B
— an international journal

Inner shell ionisation with low velocity heavy ions

Manoranjan Sarkar
Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata-700 064, India
E-mail : mano@anp.saha.ernet.in

Abstract : Inner shell ionisation with protons and alphas has been studied extensively for the last few decades but data with heavy ions are really scarce. With proton or helium, the coulombic interaction between the projectile and the electron can be well treated with the existing theories but with the low velocity heavy ions with their electron clouds, the perturbation becomes stronger and the normal collision dynamics gets modified. In order to investigate this effect, we used C and O ions from the 3 MeV Pelletron at IOP Bhubaneswar in the energy range of 4–12 MeV to measure the *K*, *L* and *M* cross sections of different elements like Ge, Ag, Au, Pb and Bi. We have also measured the anisotropy and the alignment parameters of the induced ions and the results were then compared with ECPSSR theory. In the case of *L* subshells, it was observed that the Intra-shell effect plays a significant rule at such low velocities.

Keywords : Inner shell ionization, low velocity, heavy ions.

PACS No. : 34.80.Dp

Indian J. Phys. **76B** (**4**), 401–405 (2002)

I J P B
— an international journal

Recent developments in multiphoton strong-field physics

Man Mohan
Department of Physics and Astrophysics, University of Delhi, Delhi-110 007, India

Abstract : The interaction of intense laser with an atom involves the absorption or emission of many photon resulting excitation or ionization. Perturbation theories are quite successful in explaining various multiphoton experiments. When laser intensities, $I \gtrsim 10^{13}$ W/cm^2 and infrared frequencies are employed, then free electrons are dressed by interaction. Energies which exceed the photon energies. New non-perturbative multiphoton phenomenon then occur such as above threshold ionization (ATI) and higher harmonic generation (HHG). For higher intensities $I \gtrsim 10^{16}$ W/cm^2 the electron field of laser radiation becomes greater than the coloumb-binding potential of the outer shell electron of the atom, resulting over-the-barrier ionization. With recent progress in ultrafast-optics, the intensities of the laser has been continuously increasing and now the laser intensity up to $I \approxeq 10^{20}$ W/cm^2 is available. For such high intensities, stabilization of an atom against ionization is predicted recently and involves the formation of extended wave packet of the bound state which has little overlap with the nucleus and hence a low ionization rate.

Keywords : Multiphoton, intense Laser, excitation, ionisation, atom.

PACS No. : 33.80.Rv

Indian J. Phys. **76B** (**4**), 407–414 (2002)

I J P B
— an international journal

Does hyperfine quenching affect significantly the $^3P^0_2$ level in He-like vanadium ?

T Nandi
Nuclear Science Center, Aruna Asaf Ali Marg, New Delhi-110 067, India
E-mail : nandi@nsc.ernet.in

Abstract : Using a new method of the beam-foil time-of-flight technique with a single, as well as a two-foil target, we determined the lifetime of the auto-ionizing $1s2s2p\ ^4P^0_{5/2}$ level in Li-like vanadium as 123 ± 19 ps. By accounting for the presence of the unresolved $1s^22s^2S_{1/2} - 1s2s2p\ ^4P^0_{5/2}$ satellite line in the M2 $1s^2\ ^1S_0 - 1s2p\ ^3P_2^0$ line, we deduce a lifetime of 314 ± 30 ps for the $1s2p\ ^3P_2^0$ He-like vanadium level. This value is close to theoretical estimates without invoking hyperfine interactions into account rather than to the hyperfine quenched lifetime. It thus confirms that hyperfine quenching does not influence significantly the $1s2p\ ^3P_2^0$ level lifetime in He-like vanadium. We have further developed an impirical formula to estimate the effective lifetime of the $1s2p\ ^3P_2^0$ level if satellite is not resolved in the experiment.

Keywords : Hyperfine quenching, lifetime, beam-foil time-of-flight technique.

PACS Nos. : 34.50.Fa, 32.30.Rj, 32.80.Ys

Indian J. Phys. **76B** (**4**), 415–419 (2002)

I J P B
— an international journal

Application of multidimensional SSQM formalism to He atom

Barnali Chakrabarti
Department of Physics, K N College, Berhampore, West Bengal, India
E-mail : barnali@cucc.ernet.in

Abstract : Usually the renormalized Numerov (RN) algorithm is used to solve the set of coupled differential equations of the few body system. The straight forward approach of this algorithm to the excited states faces some serious problems of convergence in binding energy. Here we present an alternative elegant approach using multidimensional super-symmetric quantum mechanics (SSQM) where the problem of convergence is avoided by searching for the ground states of the partner potentials. Application of this formalism to the first excited $^1S^e$ state of He atom gives excellent result, showing very fast convergence.

Keywords : He atom, SSQM.

PACS Nos. : 31.20.Di, 31.20.Tz, 03.65.

Indian J. Phys. **76B** (**4**), 421–424 (2002)

I J P B
— an international journal

Energetic photoionization of neutral and ionic metal clusters

Himadri S Chakraborty and M E Madjet
Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresdon, Germany

Abstract : We show, with an example of Na_{92}, that for jellium metal clusters the interference of fast electron-waves emitted from equivalent sites on the cluster edge produces monochromatic oscillations in all photoionization observables as a function of the photoelectron momentum; the effect is equivalent to the usual dispersion phenomenon. In dealing with formalisms, a serious consequence of the inadequacy of self-interaction corrected local density-functional theory in correctly accounting for the exchange interaction is identified. We also briefly discuss the influence of the ionicity of the residual core on photospectra by considering the neutral member with $N = 58$ and and the ionic member with $N = 52$ of the Na_{58} iso-jellium series, where N is the number of valence electrons. A few final remarks on possible implications of these results on other quantum systems of delocalized electrons are made.

Keywords : Jellium cluster, photoionization, density-functional theory.

PACS Nos. : 31.15.Ew, 36.40.Cg, 36.40.Vz

Indian J. Phys. **76B** (**4**), 425–429 (2002)

I J P B
— an international journal

Line strengths and line shapes of zero-phonon absorption features in solid hydrogen

A P Mishra and T K Balasubramanian

Spectroscopy Division, Modular Laboratories, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India

E-mail : amishra@apsara.barc.ernet.in

Abstract : Molecular hydrogen for which pure rotational and rovibrational electric dipole transitions in the free states are symmetry-forbidden, exhibits an infrared spectrum in the condensed phase caused by multipolar induction. Theoretical details that are essential for the interpretation of line intensity and line shapes of zero-phonon rovibrational transitions in solid H_2 and its isotopic variants are discussed.

Keywords : Line intensity and line shape, solid hydrogen, infrared spectra.

PACS Nos. : 33.70.–w, 33.20.Ea, 78.30.Hv

Indian J. Phys. **76B** (**4**), 431–441 (2002)

I J P B
— an international journal

Physics of positronium acceptor complex formation reactions

Debarshi Gangopadhyay[*], Tapas Mukherjee[#1], Bichitra Nandi Ganguly[*] and Binayak Dutta-Roy[†]

[*]Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata-700 064, India

[#]Physics Department, Bhairab Ganguly College, Kolkata-700 056, India

[†]S N Bose National Centre for Basic Sciences, III/JD Bidhannagar, Kolkata-700 098, India

E-mail : debarshi@anp.saha.ernet.in

Abstract : Positronium (Ps) reaction rates (k) with weak Acceptors (Ac) leading to the formation of Ps-Ac complexes show several interesting features : non-monotonic temperature dependence of k (departing from the usual Arrhenius behaviour), considerable variability of k with respect to different solvents, and anomalies in response to external pressure at ambient temperature. The object of this work is to explain all these phenomena using a remarkably simple bubble model (the widely used model for the pick-off component of ortho-positronium decay in liquids), which has been revisited several times in the context and as a result smooth diffuse boundary of the bubble was suggested that yields reasonable agreement of the experimental data. The contractile force on the bubble relies much on the surface tension of the liquid, through our calculation the notion of critical surface tension emerges and enables us to explain the experimental observations satisfactorily.

Keywords : Positronium, complex formation, Arrhenius behaviour, Kramers' turnover, Bubble model, critical surface tension.

PACS No. : 36.10.Dr

Indian J. Phys. **76B** (**4**), 443–448 (2002)

I J P B
— an international journal

Channeling radiation from relativistic electrons and positrons

S V S Nageswara Rao, L N S Prakash Goteti and Anand P Pathak*
School of Physics, University of Hyderabad, Central University P.O., Hyderabad-500 046, India
E-mail : appsp@uohyd.ernet.in

Abstract : The discrete nature of transverse energy associated with channeled particle has opened new applications in accelerator and atomic physics. The spontaneous transitions among these energy levels in the transverse space lead to what is known as channeling radiation. The transverse continuum potential due to two equally spaced atomic planes governing projectile motion is assumed to be harmonic type for positrons and corresponding bound states are estimated. One-dimensional hydrogen atom model for continuum potential due to single plane is used for the case of planar channeled electrons to estimate the corresponding bound states in the transverse potential well. The obstruction effects of extended defects (with specific reference to stacking faults) are incorporated suitably to obtain initial and final populations of the eigen states. The resulting expression for radiation intensities is derived using close coupling approximation.

Keywords : Electron, positron, channeled particle, bound states, close coupling app.

PACS No. : 11.80.–m

Indian J. Phys. **76B** (**4**), 449–452 (2002)

I J P B
— an international journal

Isotope shifts in UV lines of dysprosium : confirmation and new assignments of $4f^9 5d6s6p$, $4f^9 6s^2 6p$ configurations to energy levels of Dy I

B K Ankush, M N Deo, A Venugopalan* and S A Ahmad
Spectroscopy Division, Bhabha Atomic Research Centre, Mumbai-400 085, India
E-mail : avenu@apsara.barc.ernet.in

Abstract : Isotope shifts Ds (^{160}Dy–^{164}Dy) in 21 spectral lines of neutral dysprosium atom (Dy I) in the UV region have been studied; for 19 lines isotope shifts are being reported for the first time. The high-resolution spectrum has been recorded on a Fourier Transform Spectrometer using highly enriched isotopes of dysprosium, excited in a all-metal hollow cathode lamp. Using the isotope shift data, we have deduced the term isotope shifts DT (^{160}Dy–^{164}Dy) for 16 high even- and 12 high odd-parity energy levels. The earlier assignments of some of the energy levels of Dy I to $4f^9 5d6s6p$ and $4f^9 6s^2 6p$ configurations have been confirmed and a few unassigned levels have been assigned to these configurations.

Keywords : Isotope shift, atomic spectra, lanthanide, energy level, configuration.

PACS No. : 32.30.Jc

Indian J. Phys. **76B** (**4**), 453–455 (2002)

I J P B
— an international journal

Experimental investigation of angular dependence of scattering differential cross sections in double photon Compton scattering

B S Sandhu*, M B Saddi, B Singh and B S Ghumman
Physics Department, Punjabi University, Patiala-147 002, Punjab, India
E-mail : balvir@pbi.ernet.in

Abstract : The scattering differential cross sections for double photon Compton scattering have been measured for 0.662 MeV incident gamma photons on aluminium scatterer. The two simultaneously emitted gamma photons in this higher order process are detected in coincidence using two NaI(Tl) scintillation spectrometers and 30 nsec timing electronics. Many systematic effects contributing to true events have been taken into account. The measured values of scattering differential cross section agree with theory within experimental estimated error.

Keywords : Double photon Compton scattering, scattering differential cross section, coincidence events.

PACS Nos. : 32.80.t, 78.70.a

Indian J. Phys. **76B** (**4**), 457–460 (2002)

I J P B
— an international journal

Positronium formation in helium with electron correlation effect

Sabyasachi Kar and Puspajit Mandal*
Department of Mathematics, Visva-Bharati University, Santiniketan-731 235, India
E-mail : pmandal@vbharat.ernet.in

Abstract : Effects of electron correlation on positronium formation in positron-helium collisions have been studied using first-order Born and first-order distorted-wave approximations. Two correlated bound-state wavefunctions are proposed to calculate total capture cross sections at incident positron energies from the threshold at 17.8 eV upto 2000 eV. A huge collection of cross section data is compiled using these correlated and several other no-correlation wavefunctions. Present results, as expected, indicate that the electron correlation has a profound effect on the positronium formation. The correlated wavefunction which satisfies a better cusp condition of value 0.46 seems to predict realistic cross sections at all incident energies.

Keywords : Positron, positronium, electron correlation, helium, distroted-wave and Born approximations.

PACS No. : 34.85.+x

Indian J. Phys. **76B** (**4**), 461–464 (2002)

I J P B
— an international journal

Three-body recombination at low temperature—a field theoretic approach

S Bhattacharyya*, A Roy and B Mitra
Gokhale Memorial Girls' College, Kolkata-700 020, India
E-mail : sbgcmr@cal2.vsnl.net.in

Abstract : A theoretical study of the three-body recombination (TBR) of proton and electron in presence of a spectator electron with electronic beam at near – zero temperature is presented using field theory and invariant Lorentz gauge. Contributions from Feynman diagrams of different orders give an insight into the physics of the phenomena. Recombination rate coefficient (RRC) is obtained for low lying principal quantum number n = 1 to 10.

Keywords : Three-body recombination, field theoretic calculation, Feynman diagram.

PACS No. : 37.70.+e

Indian J. Phys. **76B** (**4**), 465–467 (2002)

I J P B
— an international journal

Single photo-ionization of He—a QED approach

Sujata Bhattacharyya*, Sanchita Mitra and Jhuma Bandyopadhaya
Gokhale Memorial Girls' College, Kolkata-700 020, India
E-mail : sbgcmr@cal2.vsnl.net.in

Abstract : Present paper deals with the field theoretic study of single photo-ionization (SPI) cross sections σ_{ph} and σ_c of helium due to photoelectric effect (PEE) and Compton scattering (CS) respectively, by photons of energy lying between 0–12 keV. In this energy range, σ_{ph} gradually decreases with energy while σ_c gradually increases. There is a crossover point around 6.5 keV. Near about this crossover point, graphs of σ_{ph} and σ_c are like mirror images. For photon energy below the crossover point, $\sigma_{ph} > \sigma_c$ while above that point $\sigma_c > \sigma_{ph}$. The ratio σ_c/σ_{ph} lies between 0.3 to 1.5 in the energy range under consideration. Present results are compared with existing theoretical results.

Keywords : Single ionization, photoelectric effect, Compton effect, Feynman diagram.

PACS No. : 33.80.Rv

Indian J. Phys. **76B** (**4**), 469–471 (2002)

I J P B
— an international journal

Normal coordinate analysis of deuterated benzonitriles

A Pavan Kumar, K Sriramulu and G Ramana Rao*
Department of Physics, Kakatiya University, Vidyaranyapuri, Warangal-506 009, Andhra Pradesh, India

Abstract : A zero-order normal coordinate analysis of both in-plane and out-of-plane vibrations was made for benzonitrile, benzonitrile-p-d, benzonitrile-o-d and benzonitrile-d_5 by transferring the force constants from our earlier work. The observed and calculated frequencies agree with an average error of 10.4 cm^{-1}. On the basis of calculated potential energy distributions and eigen vectors, several assignments suggested by earlier workers have been revised.

Keywords : Normal coordinate analysis, potential energy distribution.

PACS No. : 33.20.-t

Indian J. Phys. **76B** (**4**), 473–477 (2002)

I J P B
— an international journal

Normal coordinate treatment of some pyridines

B Venkatram Reddy and G Ramana Rao*
Department of Physics, University College, Kakatiya University, Vidyaranya Puri, Warangal-506 009, Andhra Pradesh, India

Abstract : A 53-parameter modified valence force field has been obtained for pyridine, pyridine-d5 and 2,6-difluoro pyridine. The force constants have been refined using vibrational frequencies employing Overlay-least-squares technique. Eigen vectors and potential energy distributions were computed. They have been used to propose unambiguous vibrational assignments for both in-plane and out-of-plane vibrational frequencies of the three molecules. On this basis certain assignments proposed by earlier workers have been revised.

Keywords : Normal coordinate treatmart, force constants, potential energy distribution.

PACS No. : 33.20.–t

Indian J. Phys. **76B** (**4**), 479–481 (2002)

I J P B
— an international journal

Time reversal symmetry breaking superconducting states in Cuprates

Angsula Ghosh
Instituto de Fisica, Universidade de São Paulo, Caixa Postal 66318, 05315-970, São Paulo, Brazil
E-mail : angsula@fge.if.usp.br

Abstract : We study the doping and temperature dependence of the order parameter for the time reversal symmetry breaking states $d_{x^2-y^2} + is$ and $d_{x^2-y^2} + id_{xy}$ using a tight binding model that includes orthorhombic distortion and second nearest neighbor hopping, g Mixing occurs both in square lattice and in the presence of orthorhombic distortion and also for various values of $g$when studied as a function of filling. We also study the specific heat for the mixed states and the coherence length for the pure $d_{x^2-y^2}$ and d_{xy} waves.

Keywords : Order parameter, symmetry breaking, super conducting, cuprates.

PACS No. : 70.20.–z

Indian J. Phys. **76B** (**4**), 483–485 (2002)

I J P B
— an international journal

A new technique for high resolution emission spectroscopy of rare and radioactive isotopes

A P Marathe, A Venugopalan and B N Jagatap*

Laser and Plasma Technology Division and Spectroscopy Division, Bhabha Atomic Research Centre, Mumbai-400 085, India

E-mail : bnj@magnum.barc.ernet.in

Abstract : A technique for high resolution emission spectroscopy of rare and radioactive elements in normal cold laboratory conditions is described. This technique makes use of a sample size of ~100 mg, mixed with suitable carriers and loaded on a new design of an all metal and liquid nitrogen cooled hollow cathode discharge lamp. The technique has been successfully used for the high resolution spectroscopy of uranium isotopes.

Keywords : High resolution spectroscopy, hyperfine structure, isotope shifts.

PACS Nos. : 32.10.Fn, 32.30.Jc, 32.70.Jz

Indian J. Phys. **76B** (**4**), 487–490 (2002)

I J P B
— an international journal

Rovibrational matrix elements of multipole moments of the heavier isotopomers of molecular hydrogen

A P Mishra, S V N Bhaskara Rao and T K Balasubramanian*
Spectroscopy Division, Modular Laboratories, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India
E-mail : tkbala@apsara.barc.ernet.in

Abstract : Rovibrational matrix elements of the multipole moments Q_λ of D_2, T_2, HD, HT and DT for ranks $2 \le \lambda \le 11$ have been computed. Since the present calculations have been performed with the nuclear center of mass (rather than the geometric center) as the origin, the computations had to include even as well as odd values of λ for the heteronuclear species HD *etc*. unlike for their homonuclear counterparts H_2, D_2 *etc*. wherein only even can λ can occur. The results are used to correlate the absorption intensities of the zero-phonon single transitions in solid HD and D_2 to theory.

Keywords : Multipole moments, solid hydrogen, infrared spectra.

PACS Nos. : 35.20.My; 33.20.Ea; 78.30.Hv

Indian J. Phys. **76B** (**4**), 491–494 (2002)

I J P B
— an international journal

Intensity and spectral distribution of 662 keV gamma rays Compton scattered from bound electrons of tin

Bhajan Singh[1*], Jagjit Kaur[2], Gurdeep Singh[3], B S Sandhu[1] and B S Ghumman[1]

[1]Physics Department, Punjabi University, Patiala-147 002, Punjab, India

[2]SGGS Govt. College, Jandiala, Jalandhar, Punjab, India

[3]Physics Department, Punjab Agricultral University, Ludhiana, Punjab, India

E-mail : bhajan@pbi.erent.in

Abstract : The intensity and energy distribution of Compton scattered gamma rays from *K*-shell electrons of tin are determined at 662 keV at scattering angles ranging from 20 to 110 degree. Two NaI (Tl) scintillation spectrometers and a coincidence set up having 30 nsec resolving time are used to record the events. The experimental results are compared with the available experimental and theoretical data.

Keywords : Compton scattering, cross section, radiation physics, energy distribution.

PACS Nos. : 32.80.t, 78.70.a

Indian J. Phys. **76B** (**4**), 495–498 (2002)

I J P B
— an international journal

Electron impact ionization of multiply charged ion : a BE study

Krishna K Prasad*
Department of Physics, V M I College, Siwan-841 226, Bihar, India
Rakesh Ranjan
Department of Chemistry, C I College, Muzaffarpur, Bihar, India
Suresh K Shrivastawa
Department of Physics, S College, Samastipur, Bihar, India
and
Anil Kumar
Department of Physics, J P University, Chapra-841 301, Bihar, India

Abstract : Thc electron impact ionization of multi-charged positive ions has been investigated in a binary encounter approximation which includes the effect of dipole interaction. Based on the geometry of the collision of electron with the target ions the model has been modified to provide a simple analytical expression for the ionization cross section. The modified expression has been used to calculate cross sections for single ionization of doubly and triply chargcd ions of noble gas atoms. The calculated cross sections are found to agree well with the available experimental measurements, especially in the higher energy region were hard collisions are expected to dominate. Comparison with experiment also shows that inclusion of inner shell contribution should further improve our results with respect to the measured values.

Keywords : Ionization cross section, electron impact, BED model.

PACS No. : 34.80.Dp

Indian J. Phys. **76B** (**4**), 499–503 (2002)

I J P B
— an international journal

High resolution studies of A^3P_0–X^1S^+ band system of InCl

M D Saksena and M N Deo

Spectroscopy Division, Modular Laboratories, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India

E-mail : mndeo@vsnl.com

Abstract : The high resolution emission spectrum of A^3P_0–X^1S^+ transition of InCl molecule (350–370 nm) has been studied by a Fourier transform spectrometer at an apodized resolution of 0.025 cm^{-1}. The rotational structure of 1-0, 2-1, 0-0, 0-1, 1-2 and 1-3 bands belonging to the A^3P_0–X^1S^+ transition of $In^{35}Cl$ has been rotationally analyzed and accurate equilibrium rotational constants of the A^3P_0 state are reported. It has also been possible to unambiguously assign rotational lines of the 1-0, 0-0 and 0-1 bands belonging to $In^{37}Cl$ isotopomer. No perturbations have been observed as pointed out by some of the earlier workers.

Keywords : Diatomic molecule, indium monochloride, rotational analysis.

PACS Nos. : 33.20.Kf, 33.20.Lg, 33.20.Sn

Indian J. Phys. **76B** (**4**), 505–507 (2002)

I J P B
— an international journal

Transport properties of gas mixtures

Kuldip Singh
Department of Physics, Guru Nanak Dev University, Amritsar-143 005, Punjab, India
E-mail : k.dip@excite.com

Abstract : A method for estimating transport coefficients of binary and multicomponent gas mixtures has been proposed. Deviations of the results predicted are of the same order as the uncertainty in experimental measurements. Finally comments on the improved corresponding states principle have been given.

Keywords : Transport coefficients, binary and multicomponent gas mixtures.

PACS No. : 51.20.+d

Indian J. Phys. **76B** (**4**), 509–511 (2002)

I J P B
— an international journal

Relativistic calculations of positron scattering from xenon (Xe) atom

Neerja and A N Tripathi
Department of Physics, University of Roorkee, Roorkee-247 667, India
E-mail : awadhfph@rurkiu.ernet.in

Abstract : We present relativistic calculations of the differential, integrated elastic, momentum transfer, total cross sections and spin polarization parameters for positrons scattered from xenon atom using a simple optical model potential to represent interaction between positron and target atoms. In the calculation, we employ a parameter-free model potential for the correlation polarization and absorption potential as devised for positron-atom scattering. Our calculated differential cross sections compare fairly well with the experimental results.

Keywords : Relativistic calculation, positron scattering.

PACS No. : 11.80.Fv

Indian J. Phys. **76B** (**4**), 513–517 (2002)

I J P B
— an international journal

Time-dependent changes in the charge-transfer spectra of ferrocene in halocarbon solvents after photoexcitation

A Thander and B Mallik*

Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700 032, India

E-mail : spbm@mahendra.iacs.res.in

Abstract : The time-dependent changes in the electronic absorption spectra of ferrocene in the halocarbon solvents chloroform and carbontetrachloride have been investigated after photoexcitation in nitrogen atmosphere. Photoexcitations have been made by the monochromatic light (using a Xe-source and a monochromator) in the UV range. It has been observed that the spectral responses with time after the removal of photoexcitations are opposite in nature for the two solvents $CHCl_3$ and CCl_4. While absorbance increases with time after photoexcitation in the case of $CHCl_3$, it decreases for CCl_4. Possible explanation has been offered for the above noted observation.

Keywords : Ferrocene, halocarbon solvents, photoexcitation, charge-transfer, time-dependent changes in spectra.

PACS Nos. : 3470, 8230, 8250

Indian J. Phys. **76B** (**4**), 519–522 (2002)

I J P B
— an international journal

Superelastic electron scattering from potassium atoms

Rajesh Srivastava and Sachin Saxena
Department of Physics, University of Roorkee, Roorkee-247 667, India
E-mail : sasasdph@isc.rurkiu.ernet.in

Abstract : We have carried out distorted wave (DW) calculations for the electron impact 4 ^2S–4 ^2P resonance excitation of potassium. The results for alignment and orientation parameters are obtained and compared with the very recent superelastic electron scattering measurements from the laser excited 4 ^2P states of potassium. The validity of DW method is commented upon.

Keywords : Electrons, excitation, Stokes parameters, alignment and orientation.

PACS No. : 34.80.Dp

Indian J. Phys. **76B** (**4**), 523–524 (2002)

I J P B
— an international journal

Millimeter and submillimeter wave spectral studies of $^{13}CD_2F_2$

R D'Cunha*, K Kawaguchi+ and M N Deo

Spectroscopy Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India

+Faculty of Science, Okayama University, Tsushima, Okayama 700-8530, Japan

E-mail : infrared@magnum.barc.ernet.in

Abstract : The millimeter and submillimeter wave spectrum of $^{13}CD_2F_2$ present in natural abundance in CD_2F_2 has been measured in the region 230–380 GHz. More than 100 rotational transitions in the ground vibrational state with $J \leq 25$ and $K_a \leq 7$ have been identified and assigned. The data have been subjected to a least squares fit, along with the reported microwave data, in the Watson's A-type reduced Hamiltonian to obtain rotational and quartic centrifugal distortion constants of the ground vibrational state of $^{13}CD_2F_2$.

Keywords : $^{13}CD_2F_2$, pure rotational spectra, millimeter wave.

PACS Nos. : 33.20.Bx, 33.20.Sn, 33.15.Mt

Indian J. Phys. **76B** (**4**), 525–528 (2002)

I J P B
— an international journal

High resolution spectroscopic studies of methyl acetylene : analysis of ν_6 band of CD_3CCH

R J Kshirsagar*, Geetha Rajappan and R D'Cunha

Spectroscopy Division, Modular Laboratories, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India

E-mail : rohidas@magnum.barc.ernet.in

Abstract : The high-resolution Fourier transform spectrum of the ν_6 band of CD_3CCH has been recorded at an apodized resolution of 0.004 cm^{-1}. The rotational structure in the ${}^pP$ and ${}^pQ$ subbands of $K = 5$ to 9 have been fitted with a standard deviation of 0.0006 cm^{-1} to evaluate the main localized Fermi resonance between the ν_6 (E) and ($\nu_7 + \nu_8 + \nu_{10}$) (E) levels. The parameters of both levels and the Fermi interaction parameter have been determined.

Keywords : ν_6 band of CD_3CCH, Fermi resonance, vibration-rotation spectra.

PACS Nos. : 33.20.Vq, 33.20.Ea, 33.15.Mt

Indian J. Phys. **76B** (**4**), 529–534 (2002)

I J P B
— an international journal

Design and fabrication of a TOF spectrometer and a 45°-parallel plate electrostatic analyzer

R K Mohanta, Rajesh Kumar Singh and R Shanker

Atomic Physics Laboratory, Physics Department, Banaras Hindu University, Varanasi-221 005, India

E-mail : rshanker@banaras.ernet.in

Abstract : We have designed and fabricated a Time-of-flight (TOF) spectrometer and a 45°-Parallel Plate Electrostatic Analyzer (PPEA) for their use in investigating the multiple ionization processes involved in collisions of keV-electrons with gaseous atomic/molecular targets. Details of design and characteristics of these instruments are reported and discussed. The methods of optimization of the TOF and that of the PPEA are described in detail. The typical test results obtained by using these instruments are found to yield a satisfactory performance.

Keywords : Time-of-flight spectrometer, parallel plate electrostatic analyzer.

PACS Nos. : 29.30.Aj, 39.90.+d

Indian J. Phys. **76B** (**4**), 535–536 (2002)

I J P B
— an international journal

Two-photon excitation using L^2 technique

R Kundliya, V Prasad and Man Mohan
Department of Physics and Astrophysics, University of Delhi, Delhi-110 007, India
E-mail : rkundliya@physics.du.ac.in

Abstract : Two-photon transition from 1*s*-3*s* state in hydrogen is studied using L^2 technique. Effect of frequency of the incident radiation on transition amplitude is shown.

Keywords : Two photon excitation, 1*s*-3*s* state in hydrogen, L^2 technique.

PACS No. : 32.80.Cy

Indian J. Phys. **76B** (**4**), 537–539 (2002)

I J P B
— an international journal

Computerized electronic locking system for diode laser frequency locking by saturated absorption spectroscopy of cesium

S J Gaur, S Pradhan, K G Manohar and B N Jagatap*
Laser and Plasma Technology Division, Bhabha Atomic Research Centre, Mumbai-400 085, India
E-mail : bnj@magnum.barc.ernet.in

Abstract : A computerized electronic locking system based on active feedback loop that controls the diode laser wavelength is reported. The system has been implemented for cooling and trapping of cesium atoms in a magneto optical trap.

Keywords : Laser locking, cooling and trapping of atoms, magneto-optical trap.

PACS No. : 32.80.pj

Indian J. Phys. **76B** (**4**), 541–544 (2002)

I J P B
— an international journal

Photoionization of noble gas atoms

S N Tiwary, R R Pandey and R P Roy
University Department of Physics, BRA Bihar University, Muzaffarpur-842 001, Bihar, India

Abstract : Photon impact ionization cross sections for the noble gas atoms (Ne and Ar) have been calculated in the *L–S* and *j–j* coupling schemes employing the reliable non-relativistic *R*-matrix and relativistic *R*-matrix methods in both the length and velocity gauges in the energy range of experimental data available. Comparison is made with all available experimental data as well as other theoretical results. Our present theoretical investigation clearly demonstrates that there is a good agreement between our present results and other results in the case of neon which reflects the correlation and relativity are not important in this case. In the case of Ar, the independent particle approximation breaks down. It exhibits that the multielectron correlation as well as relativity are important but interchannel interactions are more important than the intrachannel interaction for obtaining high precision results.

Keywords : Atoms, photons, photoionization.

PACS No. : 31.10.

Indian J. Phys. **76B** (**4**), 545–547 (2002)

I J P B
— an international journal

Laser cooling and trapping of cesium atoms in a magneto-optical trap

S Pradhan, A P Marathe, S J Gaur, A Venugopalan, K G Manohar and B N Jagatap*
Laser and Plasma Technology Division and Spectroscopy Division, Bhabha Atomic Research Center, Mumbai-400 085, India
E-mail : bnj@magnum.barc.ernet.in

Abstract : Laser cooling and trapping of cesium atoms using an indigenously developed magneto-optical trap is reported. The experimental set up of the trap and laser-cooling procedure adapted for cooling of cesium atoms is discussed.

Keywords : Laser cooling, magneto-optical trap, high-resolution spectroscopy.

PACS No. : 32.80.pj

Indian J. Phys. **76B** (**4**), 549–551 (2002)

I J P B
— an international journal

Theoretical elucidation of the infrared activity of "symmetry-forbidden" overtone bands of CO_2 induced by asymmetric isotopic substitution

T K Balasubramanian* and R J Kshirsagar

Spectroscopy Division, Modular Laboratories, Bhabha Atomic Research Center, Trombay, Mumbai-400 085, India

E-mail : tkbala@apsara.barc.ernet.in

Abstract : Recently, the intensities of the $2\nu_3$ band in $^{12}C^{16}O^{17}O$ and $^{12}C^{16}O^{17}O$ isotopomers of CO_2 were measured by high resolution Fourier transform spectrometry [1,2]. One may recall that in a linear and symmetric triatomic molecule *XYX*, the states corresponding to the vibrations ν_1, $2\nu_1$, $2\nu_3$ *etc*. are symmetry-forbidden for i.r. absorption and that their weak i.r. activity in the asymmetric isotopomer results from the mass disparity in the two isopotic atoms. The problem of quantifying the infrared activity of these forbidden bands is tractable under the Born-Oppenheimer approximation. In the present paper a theoretical framework for approaching the intensity problem is discussed in the context of the overtone band $2\nu_3$. This analysis is essentially a natural extension of our previous work [3] dealing with the mass asymmetry-induced infrared (Raman) activity of the fundamental ν_1 (ν_3). In particular, the present theory enables us to calculate, *ab initio*, the transition moment ratio $|m(2\nu_3, {}^{12}C^{16}O^{17}O)/m(2\nu_3, {}^{12}C^{16}O^{18}O)|$. The theoretical ratio compares well with the experimentally deduced value.

Keywords : Overtone bands of CO_2, infrared activity, transition dipole moments.

PACS Nos. : 33.70.Ed, 33.70.Ca, 33.20.Ea

Indian J. Phys. **76B** (**4**), 553–557 (2002)

I J P B
— an international journal

Synchronization in chaotic Jerk dynamical systems

V Patidar and K K Sud
Department of Physics, College of Science Campus, M. L. Sukhadia University, Udaipur-313 002, India
E-mail : vinodpatidar@usa.net

Abstract : In this communication we have discussed the synchronization of chaos in *Jerk dynamical system.* We have in particular applied three techniques for synchronization of chaos namely : (i) complete replacement (CR), (ii) feed back and (iii) adaptive control techniques (ACA). The stability of the synchronization in all the aforesaid methods have been discussed in detail.

Keywords : Synchronization, chaos, jerk equation.

PACS No. : 05.45.+b

Indian J. Phys. **76B** (**4**), 559–561 (2002)

I J P B
— an international journal

Incoherent scattering functions of some medium and heavy elements at 4.808 A^{-1} photon momentum transfer

N Govinda Nayak, Gerald Pinto and K Siddappa*

Department of Studies in Physics, Mangalore University, Mangalagangotri-574 199, Mangalore, Karnataka, India

*Vice Chancellor, Bangalore University, Jnanabharathi, Bangalore-560 056, India

E-mail : ncrolunayak@yahoo.com

Abstract : Whole atom differential incoherent scattering cross sections for 84.3 keV gamma photons have been measured for nine elements Cu, Mo, Ag, Cd, Sn, Ta, W, Th and U for 90° scattering of 84.3 keV gamma rays corresponding to the photon momentum transfer value X = 4.080 A^{-1}. A 100 cc HpGe detector coupled to a PC based 4K analyser was used to detect and record scattered gamma photons. From the measured cross sections the incoherent scattering functions $S(x, Z)$ were evaluated and compared with the recent experimental values reported in literature and also with the latest theoretical computations based on Hartree-Fock and Thomas-Fermi atomic model predictions. Possible conclusions are drawn on electron binding and other effects.

Keywords : Incoherent, scattering, photon.

PACS No. : 34.10.+x

Indian J. Phys. **76B** (**4**), 563–564 (2002)

I J P B
— an international journal

Two-photon ionization using pseudostate summation technique

R Kundliya, K Batra and Man Mohan
Departmant of Physics and Astrophysics, University of Delhi, Delhi-110 007, India
E-mail : rkundliya@physics.du.ac.in

Abstract : Accurate and powerful pseudostate summation technique has been used to study two-photon ionization of an atom. Results are obtained for the two-photon ionization of hydrogen from the ground state and the variation of ionization cross section on the frequency of incident radiation is shown for both linearly and circularly polarised light.

Keywords : Ionisation, pseudostate.

PACS No. : 32.80.Rm

Indian J. Phys. **76B** (**4**), 565–568 (2002)

I J P B
— an international journal

Time evolution of SERS of *a*-bithiophene and *a*-terthiophene adsorbed on Ag-sols

Uttam K Sarkar* and T N Misra
Departmant of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700 032, India

Abstract : Time evolution of Surface Enhanced Raman Spectra of *a*-bithiophene (2*T*) and *a*-terthiophene (3*T*) adsorbed on Ag-sol has been reported. Solvent effect is discussed. Orientation of the molecules in the adsorbed state is observed to control the rate of the adsorption process. Concentration dependence of time evolution is investigated. It is shown that the adsorption on the silver surface through the S atom of the oligothiophenes is a quicker process than through the *p* electrons.

Keywords : Ag-sols, oligothiophenes, surface Enhanced Raman Scattering, time evolution, solvent effect, orientation, adsorbed state.

PACS No. : 82.80.G

Indian J. Phys. **76B** (**4**), 569–572 (2002)

I J P B
— an international journal

Theoretical total cross sections of e-H_2O collisions in water, ice and dimer forms

K N Joshipura*, Minaxi Vinodkumar†, B K Antony* and C G Limbachiya‡

*Department of Physics, Sardar Patel University, Vallabh Vidyanagar-388 120, India

†V.P. & R.P.T.P. Science College, Vallabh Vidyanagar-388 120, India

‡P. S. Science College, Kadi (N. Guj.)-382 375, India

E-mail : knjoshipura@yahoo.com

Abstract : We have calculated various inelastic (including ionizing) collision parameters for the impact of electrons on H_2O molecules in the liquid (water), ice as well as cluster environments. Corresponding to incident energies E_i above the ionization threshold upto about 2000 eV, an imaginary part of complex optical potential is employed to obtain total inelastic cross sections $Q_{\rm inel}$, and these are used to derive the total ionization cross sections $Q_{\rm ion}$. The present calculations are extended to obtain the bulk or the macroscopic cross sections $\Sigma_{\rm tot}$ and the inelastic electron mean free path L as functions of energy E_i. The present results are compared with other available data.

Keywords : Electron scattering, ionization, total cross sections, macroscopic cross sections.

PACS Nos. : 61.80F, 34.90

Indian J. Phys. **76B** (**4**), 573–576 (2002)

I J P B
— an international journal

Ionized helium induced ionization of atomic hydrogen

S Bhattacharya[1], S Sahoo[*], R Das and K Roy

Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700 032, India

[1]Department of Physics, Surendra Nath College, Kolkata-700 009, India

E-mail : tpkr@mahendra.iacs.res.in

Abstract : Total and differential ionization cross sections of atomic hydrogen by impact of ionized helium in the energy range between 28 to 114 keV have been reported. We have applied a perturbative approach which accounts for the distortion due to the Coulomb fields of the projectile as well as of the residual target on equal footing. The present results, on comparing with the other existing theoretical predictions and measured data, are found to be encouraging.

Keywords : Atomic hydrogen, ionization by impact of structured projectile (He^+), calculations for collision energies 28 to 114 keV.

PACS No. : 34.50.Fa

Indian J. Phys. **76B** (**4**), 577–580 (2002)

I J P B
— an international journal

Correlation effects on peptide molecules

Puspitapallab Chaudhuri and Sylvio Canuto
Instituto de Fisica, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, SP, Brazil
E-mail : puspita@ift.unesp.br

Abstract : *Ab initio* methods are used to study the four possible dipeptides that can be formed from alanine and glycine in gas phase. We calculate the geometry, binding energy and rotational spectra of alanylalanine, alanylglycine, glycylalanine and glycylglycine. The geometries are optimized using Hartree-Fock (HF) and second-order Moller-Plesset perturbation theory (MP2). Single-point energy calculations with high-level CCSD(T) are performed on MP2 geometries. Both electron correlation and zero-point vibrational energy corrections are found to be very important and increase the calculated binding energy. Most of the correlation effects are obtained in second-order. The inclusion of zero-point correction is found to be essential.

Keywords : Correlation effects, peptide molecules.

PACS No. : 33.15.Ry

Indian J. Phys. **76B** (**4**), 581–583 (2002)

I J P B
— an international journal

Elastic scattering of electrons from methane molecule

Neerja, A N Tripathi and A K Jain[1]
Department of Physics, University of Roorkee, Roorkee-247 667, India
E-mail : neerudph@rurkiu.ernet.in

Abstract : Here we present our theoretical results for the differential scattering cross section and spin polarization parameters for elastic scattering of electrons from methane molecule at 100.00 eV using relativistic Dirac equation. The calculated spin polarization parameters are compared with those for iso-electronic neon and atomic carbon. The calculated angular distribution is compared with available experimental data.

Keywords : Elastic scattering, relativistic Dirac eqs., spin polarization.

PACS No. : 34.80.Bm