ИНСТИТУТ ЗА ФИЗИКУ

ПРИМЉЕНО: 19. 04. 2022			
Рад.јед.	број	Арх.шифра	Прилог
0801	441/1		

НАУЧНОМ ВЕЋУ
ИНСТИТУТА ЗА ФИЗИКУ
У БЕОГРАДУ

Предмет: Молба за покретање поступка за избор у звање виши научни сарадник

МОЛБА

С обзиром да испуњавам критеријуме прописане од Министарства просвете, науке и технолошког развоја за избор у звање виши научни сарадник, молим Научно веће Института за физику у Београду да покрене поступак за мој избор у наведено звање.

У прилогу достављам:

1. Мишљење руководиоца пројекта са предлогом чланова комисије за избор у звање;
2. Стручну биографију;
3. Преглед научне активности;
4. Елементе за квалитативну оцену научног доприноса;
5. Елементе за квантитативну оцену научног доприноса;
6. Списак објављених научних радова и фотокопије радова објављених након претходног избора у звање;
7. Податке о цитираности;
8. Решење о претходном избору у звање.
9. Доказе о испуњености наведених квалитативних услова

У Београду,

19.04.2022.

С поштовањем,

Jelena Maljković

Јелена Маљковић

ИНСТИТУТ ЗА ФИЗИКУ

ПРИМЉЕНО:

Рад.јед.	број	Арх.шифра	Прилог

НАУЧНОМ ВЕЋУ
ИНСТИТУТА ЗА ФИЗИКУ
У БЕОГРАДУ

Предмет: Молба за покретање поступка за избор у звање виши научни сарадник

МОЛБА

С обзиром да испуњавам критеријуме прописане од Министарства просвете, науке и технолошког развоја за избор у звање виши научни сарадник, молим Научно веће Института за физику у Београду да покрене поступак за мој избор у наведено звање.

У прилогу достављам:

1. Мишљење руководиоца пројекта са предлогом чланова комисије за избор у звање;
2. Стручну биографију;
3. Преглед научне активности;
4. Елементе за квалитативну оцену научног доприноса;
5. Елементе за квантитативну оцену научног доприноса;
6. Списак објављених научних радова и фотокопије радова објављених након претходног избора у звање;
7. Податке о цитираности;
8. Решење о претходном избору у звање.
9. Доказе о испуњености наведених квалитативних услова

У Београду,

19.04.2022.

С поштовањем,

Jelena Maljkovic

Јелена Маљковић

ИНСТИТУТ ЗА ФИЗИКУ

ПРИМЉЕНО: 19. 04. 2022

Рад.јед.	број	Арх.шифра	Прилог
0801	441/2		

НАУЧНОМ ВЕЋУ

ИНСТИТУТА ЗА ФИЗИКУ

У БЕОГРАДУ

Предмет: Мишљење руководиоца за избор др Јелене Маљковић у звање виши научни сарадник

Др Јелена Маљковић запослена је у Лабораторији за атомске сударне процесе Института за физику у Београду. У претходном периоду била је ангажована на пројектима основних истраживања Министарства просвете, науке и технолошког развоја као и на неколико међународних пројеката у оквиру којих је учествовала у екперименталним истраживањима интеракције електрона са биомолекулима, анестетицима, органометалицима као и интеракцији електрона са нанокапикларама.

С обзиром да испуњава све критеријуме прописане Правилником о поступку, начину вредновања и квантитативном исказивању научноистраживачких резултата Министарства просвете, науке и технолошког развоја, сагласан сам са покретањем поступка за избор др Јелене Маљковић у звање виши научни сарадник.

Предлажем да комисију за избор др Јелене Маљковић у звање виши научни сарадник чине:

1. др Ненад Симоновић, научни саветник, Институт за физику у Београду,
2. др Владимир Срећковић, научни саветник, Институт за физику у Београду,
3. др Братислав Маринковић, научни саветник у пензији, Институт за физику у Београду и
4. проф. др Горан Попарић, редовни професор, Физички факултет, Универзитет у Београду

У Београду,

19. 04. 2022

Руководилац лабораторије,

N. Simonović

Др Ненад Симоновић

научни саветник

Институт за физику у Београду

1. Биографски подаци

Јелена (Божидара) Маљковић је рођена у Травнику (Босна и Херцеговина) 24.04.1977. године. Физички факултет, смер Теоријска и експериментална физика, је завршила 2006. године на Универзитету у Београду са средњом оценом 8.82. Мастер студије је уписала 2006. године на Физичком факултету универзитета у Београду и завршила 2007. године са просечном оценом 10.00. Докторске студије је уписала 2007. године на Физичком факултету Универзитета у Београду – смер Експериментална физика атома и молекула и завршила са средњом оценом 10.00.
Јелена Маљковић је добитник Норвешке стипендије 2001. године.
У радном односу на Институту за физику Универзитета у Београду је од јуна 2008. године.

Учешће на националним пројектима:

2011-2019 "Физика судара и фотопроцеса у атомским, (био)молекулским и нанодимензионим системима" **No OI 171020**

2006 - 2010 “Electron and laser spectrometry and collisional cross sections for atoms, ions, molecules, metastables and biomolecules” Министарство Науке и Технолошког Развоја, Репблика Србија, **No.141011**;

Учешће на билатералним пројектима:

2016 - 2018 Република Србија – Италија, Research projects of particular relevance (Grande Rilevanza) selected within the frame of the executive programme of scientific and technological cooperation between Italian Republic and Republic of Serbia – Research area: Mathematics, Physics, Chemistry and Biology: “A nanoview of radiation-biomatter interaction”

2013 - 2015 Билатерална сарања, Српска Академија Наука и Уметности и Мађарска Академија Наука: "Interactions of charge particles with single insulating capillaries"

2012 - 2013 “Photon and electron spectroscopy of pure and nano-solvated biomolecules isolated in gas phase” Република Србија - Француска, Програм “Павле Савић” # 680-00-132/2012-09/06

2010 - 2012 “Excitation and fragmentation of small biomolecules”, Република Србија – Словачка, Билатерална сарадња No. SKSRB-0011-09.

2008 - 2009 “Electron induced fragmentation of organic molecules and small hydrocarbons”, Република Србија–Словенија, Билатерална сарадња

У оквиру ових пројеката Јелена Маљковић је значајно проширила своје знање и искуство током научних посета Институту Јожеф Штефан у Љубљани, Comenius Универзитета у Братислави, SOLEIL синхротрону поред Париза, Института Атомки у Мађарској.

Учешће на интернационалним пројектима:

- Јелена Маљковић је била члан менаџмент комитета COST акције CM1301 “Chemistry for Electron-Induced Nanofabrication (CELINA)” CSO Start of Action: 23/10/2013, End of Action: 23/10/2017.
- Кандидаткиња је учесник COST акције CA18212 “Molecular Dynamics in the GAS phase”, Start of Action - 12/11/2019 End of Action - 11/11/2023
- Кандидаткиња је учесник COST акције CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” Start of Action - 04/10/2021 End of Action - 03/10/2025

У оквиру националног пројекта ОИ171020, Физика судара и фотопроцеса у атомским, (био)молекулским и нанодимензионим системима, др Јелена Маљковић је руководилац пројектним задатком: Проучавање електронске интеракције са биомолекулима, анестетицима и наночестицама.

Јелена Маљковић је била руководилац мастер рада Јелене Вуковић а сад је руководилац докторске тезе кандидаткиње.

2. Преглед научне активности др Јелене Маљковић

Научна активност др Јелене Маљковић везана је за област атомске, молекулске и хемијске физике. Експериментална истраживања кандидаткиње се могу поделити у следеће подтеме:

1) мерење апсолутних диференцијалних пресека за еластично расејање електрона средњих енергија (40-300eV) на: биомолекулима, анестетицима и племенитим гасовима
2) трансмисију електрона средњих енергија кроз металне капиларе.
3) процесе дисоцијативног електронског захвата и дисоцијативне јонизације на органометалицима.

Напомена: Звездицом (*) су означени радови објављени након предходног избора у звање.

2.1 Мерење апсолутних диференцијалних пресека

Истраживање интеракција електрона са молекулима под добро дефинисаним експерименталним условима има за циљ да се прошири знање о молекулским процесима (разумевање структуре и динамике молекулских система) како би се исти могли карактеризовати у теоријским прорачунима. Налажење вероватноће, тј. диференцијалног пресека је од пресудног значаја за опис сударног процеса и у експерименталним и у теоријским истраживањима. Експериментално одређивање диференцијалног пресека заснива се на мерењу интензитета, тј. броја расејаних електрона у функцији угла или енергије при чему између мереног сигнала и траженог пресека постоји директна зависност. У оквиру истраживања електронских сударних процеса били су одређивани релативни и апсолутни диференцијални пресеци за еластично расејање електрона средњих енергија, од 40-300eV на биомолекулима (аналогним неким деловима ДНК), анестетицима, метану и аргону. Сва мерења су извршена у режиму бинарних судара техником укрштених млазева – електронског млаза произведеног у електронском топу и млаза молекула.
Од 2007 године кандидаткиња се бавила проучавањем интеракције електрона средњих енергија са биомолекулима аналогним неким деловима ДНК. Наставак на предходно мерене молекуле који су аналогни неким деловима молекула релевантним за грађу биолошких макромолекула: фуран, 3 hидрокситетрахидро фуран (аналогни дезоксирибози у ДНК), пиримидин (аналоган пиримидинским базама), формамид и н-метилформамид (молекули који садрже пептидну везу), је било мерење релативних и апсолутних диференцијалних пресека за еластично расејање електрона на триетил фосфату $(C_2H_5)_3PO_4$ који је аналоган фосфатној групи у ДНК. Теоријске прорачуне је радио професор Tökési iz Mađarske.
Резултати истраживања расејања електрона на молекулима аналогним неким деловима ДНК приказани су у следећим радовима:

(M23*) Jelena B. Maljković, Jelena Vuković, Károly Tökési, Branko Predojević, and Bratislav P. Marinković,
“Elastic electron scattering cross sections for triethyl phosphate molecule at intermediate electron energies from 50 to 250 eV”,
Eur. Phys. J.D ***73****, 27 (2019). [5pp] (on-line 5 Feb 2019)*
doi: 10.1140/epjd/e2019-90631-1

(M21) J. B. Maljković, F. Blanco, R. Čurik, G. García, B. P. Marinković, and A. R. Milosavljević,
“Absolute cross sections for electron scattering from furan”,
J. Phys. Chem. ***137*** *064312 (2012) [10 pages].*
http://link.aip.org/link/?JCP/137/064312
doi: 10.1063/1.4742759

(M21) J. B. Maljković, F. Blanco, G. García, B. P. Marinković, and A. R. Milosavljević,
“Absolute cross sections for elastic electron scattering from methylformamide”,
Physical Review A ***85****, 042723 (2012) [8 pages].*
http://link.aps.org/doi/10.1103/PhysRevA.85.042723
DOI: 10.1103/PhysRevA.85.042723

(M21) J. B. Maljković, A. R. Milosavljević, F. Blanco, D. Šević, G. García, and B. P. Marinković,
“Absolute differential cross sections for elastic scattering of electrons from pyrimidine”,
Phys. Rev. A ***79****, 052706 (2009) [7 pages].*
http://link.aps.org/doi/10.1103/PhysRevA.79.052706
doi: 10.1103/PhysRevA.79.052706

(M22) J. B. Maljković, F. Blanco, G. García, B. P. Marinković, and A. R. Milosavljević,
“Elastic electron scattering from formamide molecule”,
Nucl.Instrum. Meth. B. ***279*** *124-127 (2012).*
doi:10.1016/j.nimb.2011.10.029

(M23) A. R. Milosavljević, F. Blanco, J. B. Maljković, D. Šević, G. García, and B. P. Marinković,
“Absolute cross sections for elastic electron scattering from 3-hydroxytetrahydrofuran”,
New J. Phys. ***10*** *103005 (2008) [19 pages].*
doi: 10.1088/1367-2630/10/10/103005

(M23) B. P. Marinković, A. R. Milosavljević, J. B. Maljković, D. Šević, B. A. Petruševski, D. Pavlović, D. M. Filipović, M. Terzić and V. Pejčev,
“Optical and Electron Spectrometry of Molecules of Biological Interest”,
Acta Physica Polonica A ***112****(5) 1143-1148 (2007).*

Апсолутни диференцијални пресеци мерени су и на halogenim inhalacionim анестетицима халотену ($C_2HBrClF_3$) и севофлурану $C_4H_3F_7O$). Фокусирање на упознавање молекулске структуре и хемијских особина халогених анестетика може помоћи у разумевању њихових реактивности и унапређењу у клиничкој употреби. Севофлуран се користи од 1990г а сад је један од најкоришћенијих анестетика у различитим типовима операција као и у дечијој хирургији. Такође, халогени анестетици су битни због њихове улоге у атмосферској хемији, заједно са улогом хлорофлуорокарбона у оштећењу озонског омотача у стратосфери. Инхxалациони анестетици се врло мало метаболички мењају при клиничкој употреби, тако да молекули анесатетика са дугим временом живота могу стићи у стратосферу у великој количини. Теоријски прорачуни за ова мерења су рађени од стране групе из Шпаније и јако добро имамо слагање експеримента и теорије. Резултати за халотен су приказани на неколико саопштења на међународним конференцијама а публикација рада је току.
Резултати истраживања расејања електрона на молекулима анестетика приказани су у следећим раду и саопштењу са конференције:

(M21*)Jelena Vukalović, Jelena B. Maljković,FranciscoBlanco,Gustavo García, Branko Predojević, Bratislav P. Marinković

"Absolute differential cross-sections for elastic electron scattering from sevoflurane molecule in the energy range from 50-300 eV",
Int. J. Molec. Sci. ***23****(1) 21 (2022) [11pp].*
doi: 10.3390/ijms23010021
ISSN: 1422-0067

(M33) Jelena B. Maljković, Aleksandar R. Milosavljević, Zoran Pešić, F. Blanco, G. García, Dragutin Šević and Bratislav P. Marinković

"Absolute differential cross section for elastic electron scattering from halothane at 100eV
Proc. 25th Summer School and International Symposium on Physics of Ionized Gases SPIG, 30th Publ. Astron. Obs. Belgrade No. 89, July (2010),
ISSN: 0373-3742 pp. 33 – 36.

Кандидаткиња се бавила и проучавањем метана (CH_4), гаса који у великој мери, доприноси ефекту "стаклене баште". Овај ефекат је око 8 пута већи од CH_4 него од CO_2. Метан је проучаван:

а) одређивањем апсолутих диференцијалних пресека за еластично расејање електрона на молекулима метана на електронском спектрометру УГРА на Институту за физику у Београду

б) одређивањем енергија појављивања продуката дисоцијације услед ексцитације електронима, приликом посете Comnenius факултету у Братислави у оквиру билатералне сарадње.
Резултати истраживања расејања електрона на молекулима метана приказани су у следећим радовима:

(M21*)Jelena Vukalović, Jelena B. Maljković, Karoly Tökési, Branko Predojević, Bratislav P. Marinković,
"Elastic electron scattering from methane molecule in the energy range from 50-300 eV",
Int. J. Molec. Sci. ***22****(2) 647 (2021) [14pp].*
Special Issue "Electron and Photon Interactions with Bio(Related) Molecules"
doi: 10.3390/ijms22020647
ISSN: 1422-0067

(M21)M Danko, J Orszagh, M Durian, J Kočišek, M Daxner, S Zöttl,
J B Maljković, J Fedor, P Scheier, S Denifl and Š Matejčik
"Electron impact excitation of methane:determination of appearance energies for dissociation products"
J. Phys. B: At. Mol. Opt. Phys **46** 045203 (2013)
doi: 10.1088/0953-4075/46/4/045203

Апсолутни диференцијални пресеци (DCS) за еластично расејање електрона на аргону су такође мерени на електронском спектрометру УГРА. За рефентни гас у методи Релативних протока (Relative flow) коришћен је хелијум. Овим резултатима смо добили један конзистентан скуп апсолутних диференцијалних пресека за еластчно расејање електрона на аргону за средњи распон уданих енергија (40-300eV) које смо користили као референтне пресеке за мерења апсолутних DCS свих наредних мета.

Из овог мерења публикован је рад:

(M23*)Milos Lj. Rankovic, Jelena B. Maljkovic, Karoly Tokesi, and Bratislav P. Marinkovic,
Elastic electron diferential cross sections for argon atom in the intermediate energy range from 40 eV to 300 eV
Eur. Phys. J.D 72, 30 (2018) [9pp],
doi: 10.1140/epjd/e2017-80677-4
ISSN: 1434-6060

У циљу добијања поузданих вредности пресека било је потребно развити методологију мерења и унапредити низ експерименталних техника у електронској спектрометрији. У оквиру ове тематике Јелена Маљковић је радила на:
- унапређењу гасног система апаратуре УГРА у циљу омогућавања мерења апсолутних диференцијалних пресека, *Relative flow method*. Суштина овог метода је упоредно мерење сигнала расејаних електрона за непознатом и такозваном

референтном гасу, уз додатно мерење брзине протока сваког гаса и пажљиво подешавање апсолутних притисака.

- калибрацији и тестирању експерименталног уређаја;
- методологији мерења релативних пресека и добијању апсолутних вредности диференцијалних пресека.

Енергијски разложене структуре у спектрима губитака енергије директно описује процесе ексцитације молекула. Разумевање ових структура и свеукупне интеракције електрона са органским молекулима, обезбеђује основу за разумевање како структуре тако и динамике ових система. Иако је поставка апаратуре на којој су рађена истраживања пре свега оптимизована за мерење релативних и аспсолутних диференцијалних пресека за еластично расејање електрона и не дозвољава мерење спектара губитака енергије са веома високом енергијском резолуцијом, добијени спектри су од значаја за проверу чистоће мете, као и за подршку оптичким спектрима при анализи података добијених мерењима на синхротрону са ултра-високом резолуцијом.

Резултати до којих је дошла кандидаткиња у оквиру ове тематике упоређени су са теоријским прорачунима, што је омогућило тестирање и унапређење теоријских модела и метода за одређивање апсолутних пресека за еластично расејање електрона средњих енергија на релативно великим молекулима. Добијени су вредни резултати како за фундаментално разумевање процеса интеракције елементарних честица са комплексним молекулским системима, тако и за мултидисциплинарна истраживања која могу имати важну примену у биомедицинским наукама.

2.2 Интеракција електрона са металним капиларама

Разумевање и интерпретација спектра електрона расејаних на чврстим површинама је битно за многе техничке апликације. За карактеризацију површина и дијагностику којом се избегава оштећење материјала и модификација површине као и разумевању самих процеса расејања. На експерименту УГРА кандидаткиња се бавила проучавањем трансмисије електрона кроз макроспопске металне капиларе, након вишеструких судара са зидовима мете. Јасно је да је експериментално немогуће одредити разлику између трансмитованих примарних и секундарних електрона генерасаних у нееластичним сударима са зидовима капиларе и захтева додатне симулације трансмисије.

У колаборацији са колегама из Мађарске и Винче, који су били задужени за симулације, кандидаткиња је објавила два рада.**:**

(M22*) <u>J.B. Maljković</u>, D. Borka, M. Lj. Ranković, B.P. Marinković,
A.R. Milosavljević, C. Lemell, and K. Tőkési

"Electron transmission through a steel capillary", *Nucl. Instrum. Meth. B*, **423**, 87–91 (2018).

doi: 10.1016/j.nimb.2018.03.020

ISSN: 0168-583X

(M21*) A. R. Milosavljević, M. Lj. Ranković, D. Borka, J. B. Maljković, R. J. Bereczky, B. P. Marinković and K. Tőkési

“Study of electron transmission through a platinum tube”,
Nucl. Instrum. Meth. B **354**, 86-89 (2015). [on-line 15 Dec 2014]
doi: 10.1016/j.nimb.2014.11.087
ISSN: 0168-583X

2.3 Интеракција електрона са органометалицима

FEBID (Focused Electron Beam Induced Deposition) је врло обећавајућа техника депозиције за нанофабрикацију, која производи 3Д структуре од суб-10nm димензија. Велики број органометалика произведених специјално за CVD (Chemical Vapour Deposition), FEBID користи за своје прекурсоре, за производњу 3Д металних наноструктура. FEBID је техника у којој се високоенергијски фокусирани сноп усмери на перкурсор доводећи до дисоцијације и у идеалном случају водећи ка стварању депозита.. Наиме, високоенергијски сноп ствара мноштво секундарних електрона са енергијом испод 100 eV који доводе до фрагментације прекурсора коз различите процесе декомпозиције, као што су дисоцијативна јонизација, диполарна дисоцијација, неутрална дисоцијација и процес дисоцијативног електронског захвата (DEA). У оквиру ове тематике, а у сарадњи са колегама из Словачке и Пољске, кандидаткиња је проучавала процесе дисоцијативне јонизације за tetraethyl ortosilicate (TEOS) као и процес дисоцијативног електронског захвата за TEOS и benzene chromium tricarbonil molekule. Обе мете се могу сматрати потенцијалним FEBID прекурсорима. Мерења на TEOS молекулу су извођена на две независне експерименталне поставке на, Cross Beam (CBA) и Claster Aparateus (CA), на Comnenius факултету у Братислави. Обе експерименталне поставке поседују Trohoidal Electron Monochromator (TEM) и Quadropol Mass Analyzer (QMA). Обе апаратуре користе метод укрштених млазева, млаз електрона се у интеракционој запремини под углом од 90˚ судара са млазом молекула мете. Након што се у интеракционој запремини формирају позизтивни јони, они се масено анализирају у QMA и детектују. Након налажења масеног спектра за TEOS молекул прагови енергије за стварање сваког позивног фрагмента су мерени. Током кандидаткињиног боравка у Пољској процес дисоцијативног електронског захвата на benzene chromium tricarbonyl молекулу је проучаван. Овај орaганометалик је такође потенцијални FEBID прекурсор. Такође експеримент је базиран на методи укрштених млазева, са TEM-om, QMA и детектором, смештеним у вакумску комору. Мерења су рађена у функцији енергије упадних електрона од 0-12e V. У овом енергијском распону процес дисоцијативног електронског захвата је заслужан за фрагментацију молекула. Молекул је показао врло богато формирање анјона. У оквиру потенцијалне улоге хромијумивих јединјена у FEBID-у, показано је да је DEA процесима могуће уклонити и бензен и све CO групе и формирати $[Cr]^-$. Кандидаткиња је током боравка од три недеље у Пољској, у оквиру научне посете COST акције CELINA, радила на мерењима везаним за DEA процесе на овом молекулу.

Ове резултате кандидаткиња је представила на CELINA састанцима у Братислави и Кракову и објављен је рад :

(M21[*]) Janina Kopyra, Paulina Maciejewska and Jelena Maljković

"Dissociative electron attachment to coordination complexes of
chromium: chromium(0) hexacarbonyl and benzene-chromium(0) tricarbonyl",
Beilstein J. Nanotechnol. **8**, 2257–2263 (2017).
doi: 10.3762/bjnano.8.225
ISSN: 2190-4286

(M32*) Jelena Maljković, Paulina Maciejewska and Janina Kopyra,
"Dissociative electron attachment to benzene chromium tricarbonyl"
Proc.The 3rd CELINA Meeting, Kraków, May 18-20, 2016, Eds. Petra Swiderek and
Janina Kopyra, p.20
http://celina.uni-bremen.de/celina/celina2016/index.php?id=start&lang=en

(M32[*]) Jelena Maljković, Peter Papp, Michal Lacko, Michal Stano, Aleksandar Milosavljević, Stefan Matejcik
"Electron impact dissociative ionization of tetraethyl orthosilicate",
Proc. 2nd Annual Meeting of COST Action CM 1301, CELINA - Chemistry for ELectron-Induced Nanofabrication, May 6-9, 2015, Bratislava, Slovakia, Book of Abstracts, Eds. Peter Papp and Petra Swiderek, (COST Action CM 1301, Comenius University, Bratislava, Slovakia), STSM Report, WG1, p.29.
http://neon.dpp.fmph.uniba.sk/celina2015/
Acknowledgements: grants – Slovak Research and Development Agency under Contract No. APVV-0733-11; MESTD RS OI #171020; COST Action CM1301 (CELINA).
ISBN: / (The Comenius University, Bratislava, Slovakia)

3. ЕЛЕМЕНТИ ЗА КВАЛИТАТИВНУ ОЦЕНУ НАУЧНОГ ДОПРИНОСА КАНДИДАТА

3.1 Квалитет научних резултата

3.1.1 Научни ниво и значај резултата, утицај научних радова

Јелена Маљковић је у свом досадашњем научном раду објавила укупно 14 радова у међународним часописима, једно предавање по позиву са међународног скупа штампано у целини, 5 предавања по позиву са међународних скупова штампана у изводу, 5 саопштења са међународних скупова штампана у целини, 14 саопштења са међународних скупова штампана у изводу, 2 предавање по позиву са скупа националног значаја штампана у целини, 1 саопштења са скупа националног значаја штампана у целини и 2 саопштења са скупа националног значаја штампана у изводу.

Кандидаткиња је након претходног избора у звање научни сарадник објавила 7 радова у међународним часописима са ISI листе. **Четири рада** су **категорије М21** (врхунски међународни часописи), **један** у **категорији М22,** **два** у **категорији М23**. Поред тога, објавила је **1 рад категорије М31** (предавање по позиву са међународног скупа штампано у целини), **4 рада категорије М32** (предавање по позиву са међународног скупа штампано у изводу), **2 категорије М33** (саопштење са међународног скупа штампано у целини) и **9 радова категорије М34** (саопштење са међународног скупа штампано у изводу).

Као пет најзначајнијих радова др Јелене Маљковић могуће је издвојити:

1. (M21) Jelena Vukalović, **Jelena B. Maljković**, Francisco Blanco, Gustavo García, Branko Predojević, Bratislav P. Marinković,

"Absolute differential cross-sections for elastic electron scattering from sevoflurane molecule in the energy range from 50-300 eV",

Int. J. Molec. Sci. 23(1) 21 (2022). M21=8, ИФ=5.924, цитиран 0 пута (рад је тек изашао)

2. Janina Kopyra, Paulina Maciejewska and **Jelena Maljković**,

"Dissociative electron attachment to coordination complexes of chromium: chromium(0) hexacarbonyl and benzene-chromium(0) tricarbonyl",

Beilstein J. Nanotechnol. **8**, 2257–2263 (2017), M21=8; ИФ=3.127, цитиран 5 пута

3. J. B. Maljković, A. R. Milosavljević, F. Blanco, D. Šević, G. García, and B. P. Marinković,

"Absolute differential cross sections for elastic scattering of electrons from pyrimidine",

Phys. Rev. A **79**, 052706 (2009), M21=8; ИФ =2.908, цитиран 53 пута

4. J. B. Maljković, F. Blanco, R. Čurik, G. García, B. P. Marinković, and A. R. Milosavljević,

“Absolute cross sections for electron scattering from furan”,

J. Chem. Phys. **137** 064312 (2012), М21=8, ИФ=3.164, цитиран 10 пута

5. Jelena Vukalović, Jelena B. Maljković, Karoly Tökési, Branko Predojević, Bratislav P. Marinković,
“Elastic electron scattering from methane molecule in the energy range from 50-300 eV”,
Int. J. Molec. Sci. 22(2) 647 (2021) . М21=8, ИФ=5.924, цитиран 1 пут

У првом раду објављеном у *International Journal of Molecular Sciences **23**(1) 21 (2022)* су приказани теоријски и експериментални апсолутни диференцијални пресеци за еластично расејање електрона на молекулима севофлурана, једног од најчешће коришћених халогених анестетика. Интересовање за проучавање анестетика у последње време је порасла и са чињеницом да халогени анестетици су битни због њихове улоге у атмосферској хемији, заједно са улогом хлорофлуорокарбона у оштећењу озонског омотача у стратосфери. Инххалациони анестетици се врло мало метаболички мењају при клиничкој употреби, тако да молекули анесатетика са дугим временом живота могу стићи у стратосферу у великој количини. Експериментални и теоријски резултати се јако добро слажу на апсолутној скали, што говори о поузданости наше експерименталне методе.

У другом раду објављеном у *Beilstein J. Nanotechnol.* **8**, 2257–2263 (2017), смо разматрали на примеру молекула $Cr(CO)_6$ и $(\eta_6\text{-}C_6H_6)Cr(CO)_3$ како замена три CO групе са C_6H_6 има утицаја у случају интеракције ових молекула са електронима. Кандидаткиња је овај рад објавила током научне посете Пољској у оквиру COST акције CELINA. У оквиру потенцијалне улоге хромијум једињења у FEBID апликацијама утврдили смо да ″откидање″ C_6H_6 и свих CO лиганада и формирање чистог $[Cr]^-$ је могуће путем процеса дисоцијативног електронског захвата.

У трећем раду објављеном у *Phys. Rev. A **79**, 052706 (2009)* смо приказали теоријска и експериментална истраживања еластичног расејања електрона на пиримидину, молекулу који је аналоган пиримидинским базама. Мерења су рађена на упадним енергија 50-300 eV и упадним угловима 20º-110º. Релативни диференцијални пресеци су мерени у функцији угла и упадне енергије електрона и нормирани су на апсолутну скалу на основу тачака добијених Relative flow методом. Теоријски прорачуни су базирани на коригованој форми метода независних атома (Inedependent Atom Methode-IAM).

У четвртом раду објављеном у *J. Chem. Phys.* **137** 064312 (2012), приказани су резултати за фуран молекул, апсолутни пресеци у функцији угла за енергије 50-300 eV, 20°-110°, табеларно и графички. Ови апсолутни пресеци у функцији угла су упоређени са SCARND i UFBA теоријом, као и са ранијим експерименталним резултатима. На примеру молекула фурана, у сарадњи са колегом Р. Чуриком из Прага, разматран је утицај вибрационих стања која се не могу у експерименту раздвојити од еластичног расејања на средњим енергијама. Дат је такође график ротационо сумираних вибрационих нееластичних апсолутних пресека и односа суме вибрационих нееластичних апсолутних пресека према еластичним. На крају су представљени, графички и табеларно, интегрални и тотални пресеци и упоређени са ранијим резултатима.

У петом раду објављеном у *International Journal of Molecular Sciences* **22**(2) 647 (2021) су презентовани експериментално добијени диференцијални пресеци за еластично расејање електрона на метану (CH_4), гасу који у великој мери, доприноси ефекту "стаклене баште". Експериментални резултати су упоређени са два сета теоријских података једним добијеним обичном сумом инвидуалних атома а другим добијеним узимајући и ефекте молекула у обзир. Експериментални и теоријски резултати се добро слажу на апсолутној скали и са предходно добијеним резултатима других аутора, што говори и о поузданости наше експерименталне методе и теоријског метода.

3.1.2 Позитивна цитираност научних радова кандидата

Према бази Web of Science, радови др Јелене Маљковић укупно су цитирани 154 пута, док је број цитата без аутоцитата 132. Хиршов индекс је h=7.

Прилог: подаци о цитираности радова из интернет базе Web of Science

3.1.3 Параметри квалитета радова и часописа

Као битан елемент за процену квалитета научних радова служи и импакт-фактор

часописа у којима су радови објављени.

Од предходног избора у звање кандидаткиња је објављивала радове у часописима категорија M21, M22 i M23 :

Категорија M21:

2 рада у *International Journal of Molecular Sciences*, Impact Factor (5.924)

1 рада у *Nucl. Instrum. Meth. B,* Impact Factor (1.389)

1 рад у Beilstein J. Nanotechnol, Impact Factor (3.127)

Категорија M22:

1 рад у Nucl. Instrum. Meth. B, Impact Factor (1.210)

Категорија M23:

1 рад у Eur.Phys.J.D., Imact factor (1.288)

1 рад у Eur. Phys. J.D , Impact Factor (1,288)

Укупан импакт фактор ових радова је **20.15.**

Часописи у којима објављује др Јелена Маљковић су цењени по свом угледу и водећи у његовим областима рада. Додатни библиометријски показатељи према упутству о начину писања извештаја о изборима у звања које је усвојио Матични научни одбор за физику приказани су у следећој табели:

	ИФ	М	СНИП
Укупно	20,15	43	6.947
Усредњено по чланку	2.88	6.14	0.992
Усредњено по аутору	3.964	8.53	1.353

3.1.4 Степен самосталности и степен учешћа у реализацији радова у научним центрима у земљи и иностранству

Од 14 објављених радова, др Јелена Маљковић је први аутор на 7 радова. На радовима који су објављени у периоду након одлуке Научног већа Института за физику о предлогу за стицање претходног научног звања, кандидаткиља је објавила 7 радоva и први је аутор на 2 рада.

При изради поменутих публикација кандидаткиња је учествововала у осмишљавању мета коришћених за истраживање, експеерименталним мерењима, на обради и анализи добијених резултата и писању радова.

Током докторских студија, под менторством др Александра Милосављевића с Института за физику у Београду, др Јелена Маљковић је започела истраживање у области радијационог оштећења живе материје, под утицајем електрона средњих енергија (40-300 eV). У том контексту, проширено је експериментално истраживање интеракције електрона средњих енергија са молекулима који су аналогни неким деловима ДНК. Зазапочет је развој методе за мерење апсолутних диференцијалних пресека (Relative flow метод) за еластично расејање електрона на биомолекулима, аналогним неким деловима молекула релавантним за грађу биолошких макромолекула. Након завршеног доктората, кандидаткиња је наставила да се бави проблемом интеракције електрона средњих енергија са биомолекулима и започела је рад на интеракцији електрона средњих енергија са анестетицима, метану и металним капиларама. У оквиру националног пројекта OI 171020 Физика судара и фотопроцеса у атомским, (био)молекулским и нано система, руководилац је пројектног задатка:

Проучавање електронске интерације са (био)молекулима, анестетицима и наночестицама. Поред ових тема, у сарадњи са колегама из Словачке и Пољске, кандидаткиња се бавила проучавањем процеса дисоцијативне јонизације и дисоцијативног електронског захвата на органометалицима који су потенцијални FEBID прекурсори. У оквиру COST акције CELINA кандидаткиња је у више наврата боравила у Словачкој и Пољској, где је остварила научну сарадњу са проф др Штефаном Матејчиком, др Петром Пап и проф др Јанином Копиром . Из ове сарадње објављена су два рада и одржана два предавања ма међународним конференцијама.

3.1.5. Елементи примењивости научних резултата

Резултати радова са биомолекулима су значајни у циљу изучавања директог оштећења биолошког материјала услед дејства јонизујућег зрачења. Експерименти у којима се истражује процес интеракције електрона са молекулима који су аналогни градивним деловима ДНК и протеина су зато јако битни. Спектроскопски подаци и апсолутни диференцијални пресеци за интеракцију електрона са ДНК су потребни као почетни параметри у моделовању процеса оштећења и разумевању реакција. Добијање диференцијалних ефикасних пресека за расејање електрона на биомолекулима је важно за тестирање теоријских модела који се примењују за прорачун сударних процеса. Такође поуздано измерени диференцијални пресеци представљају важне улазне параметре за Monte Carlo симулације депозиције енергије у живој материји услед дејства јонизујућег зрачења. Треба истаћи да је поуздан прорачун радијационог оштећења произведеног високоенергијским честицама битан део истраживања повеазаног са канцер терапијом.

Резултати радова са органометалицима имају значајне примене како су органометалици велика група једињења са бројним апликацијама у фармацеутској индустрији и нанотенологији. Велики број органометалика су препознати као обећавајући прекурсори за Focused Electron Beam Induced Deposition (FEBID), процесе за фабриковање три-димензионалних металних наноструктура.

3.2 Ангажованост у формирању научних кадрова

Кандидаткиња је била ментор на изради мастер рада Јелене Вуковић (сад Вукаловић), одбрањеног 2018-те године. Др Јелена Маљковић је тренутно ментор на докторским студијама Јелене Вуковић (Вукаловић),

Прилог: потврда о менторству на мастер и докторским студијама

3.3 Нормирање броја коауторских радова, патената и техничких решења

Сви радови кандидаткиње објављени након одлуке Научног већа Института за физику о предлогу за стицање претходног научног звања укључују резултате експерименталног истраживања интеракције електрона са биомолекулима, анестетицима, метану, металним капиларама и органометалицима. Од тога, сви радови имају мање или 7 коатора, тако да улазе пуном тежином. Укупан број поена М поена др Јелене Маљковић у релевантном периоду, од предходног избора у звање, износи 59 што је изнад захтеванох броја бодова за избор у звање виши научни сарадник..

3.4 Руковођење пројектима, потпројектима и пројектним задацима

У оквиру националног пројекта ОИ171020 , Физика судара и фотопроцеса у атомским, (био)молекулским и нанодимензионим системима, др Јелена Маљковић је руководилац пројектним задатком: Проучавање електронске интеракције са биомолекулским, анестетицима и наночестицама.

Прилог: потврда вође пројекта о руковођењу наведеним пројектним задатком.

3.5 Активност у научним и научно-стручним друштвима

- Др Јелена Маљковић је члан Одељења Друштва физичара Србије за научна истраживања и високо образовање у Одсеку за атомску и молекулску физику.
- Кандидаткиња је била члан менаџмент комитета COST акције CM1301 “Chemistry for Electron-Induced Nanofabrication (CELINA). Approval date: 16/05/2013, End of Action: 15/05/2017.

  Прилог: записник са седнице Научног већа, позив CELINA акције за чланство у менаџмент комитету акције.
- Кандидаткиња је заменик члана менаџмент комитета COST акције CA18212 “Molecular Dynamics in the GAS phase”, Start of Action - 12/11/2019 End of Action - 11/11/2023

  Прилог : позив MD COST акције за заменика члана менаџмент комитета
- Кандидаткиња је учесник COST акције CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” Start of Action - 04/10/2021 End of Action - 03/10/2025

  Прилог : позив акције CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” за чланство

3.6 Утицајност научних резултата

Утицај научних радова кандидаткиње детаљно је приказан у одељку 3.1 овог документа **Квалитет научних резултата.**

3.7 Конкретан допринос кандидата у реализацији радова у земљи и иностранству

Др Јелена Маљковић је значајно допринела сваком раду у чијој припреми је учествовала. Од 7 радова објављених у периоду након одлуке Научног већа Института за физику о предлогу за стицање претходног научног звања, сви радови су урађени у сарадњи с колегама из земље и иностранства. Кандидаткиња је у овим радовима имала кључни допринос: на 2 рада је први аутор, а на 3 рада је наведена као други аутор а на једном као последњи. Током израде ових публикација, она је радила на осмишљавању мета интересантних за истраживања, експерименталним мерењима, обради и анализи резултата и писању радова. Знања и искуства које је стекла у експерименталном раду и обради података добијених у експерименталним истраживањима кандидаткиња преноси млађим сарадницима у Лабораторији за атомске сударне процесе.

3.8 Уводна предавања на конференцијама и друга предавања

Након претходног избора у звање, др Јелена Маљковић је одржала следећа предавања по позиву:

1. 6th Conference on Elementary Processes in Atomic Systems – CEPAS 2014, 9th - 12th July 2014, Bratislava, Slovakia.
2. 27th Summer School and International Symposium on the Physics of Ionized Gases – SPIG 2014, 26-29 August 2014, Belgrade, Serbia.
3. 2nd Annual Meeting of COST Action CM 1301, CELINA - Chemistry for ELectron-Induced Nanofabrication, May 6-9, 2015, Bratislava, Slovakia.
4. 3rd Annual Meeting of COST Action CM 1301, CELINA - Chemistry for ELectron-Induced Nanofabrication, May 18-20, 2016, Kraków, Poland
5. Атомско-молекуларне базе података, Тренинг, 23.11.2017, Универзитет у Бањој Луци ОЈ Природно-математички факултет
6. 7th International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces ¬ MPS2018, 21-24 August 2018, Budapest, Hungary,
7. 1st General Meeting of the COST Action: MD-GAS (Molecular Dynamics in the GAS-phase). February 18-21, 2020. Caen, France

Прилог: позиви за предавања, позив за предавање на првом MD GAS конференцији, MPS конференцији, распоред предавача са CELINA састанка у Братислави, позив за предавање у Бања Луци

Елементи за квантитативну аналаизу научног доприноса

Остварени М-бодови кандидата по категоријама публикација:

Категорија	М бодова по раду	Број радова	Укупно М бодова	Нормализовано М бодова
M21	8	4	32	32
M22	5	1	5	5
M23	3	2	6	6
M31	3.5	1	3.5	3.5
M32	1.5	4	6	6
M33	1	2	2	2
M34	0.5	9	4.5	4.5

Поређење оствареног броја М-бодова са минималним условима потребним за избор у звање виши научни сарадник:

Минималан број М бодова		Остварено	Остварено (нормализовано)
Укупно	50	59	59
M10+M20+M31+M32+M33+M41+M42	40	54.5	54.5
M11+M12+M21+M22+M23	30	43	43

УКУПАН СПИСАК НАУЧНИХ РАДОВА

МОНОГРАФИЈЕ, МОНОГРАФСКЕ СТУДИЈЕ, ТЕМАТСКИ ЗБОРНИЦИ, ЛЕКСИКОГРАФСКЕ И КАРТОГРАФСКЕ ПУБЛИКАЦИЈЕ МЕЂУНАРОДНОГ ЗНАЧАЈА

M14

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B. P. Marinković, V. Pejčev, D. M. Filipović, D. Šević, A. R. Milosavljević, S. Milisavljević, M. S. Rabasović, D. Pavlović and J. B. Maljković
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РАДОВИ ОБЈАВЉЕНИ У НАУЧНИМ ЧАСОПИСИМА МЕЂУНАРОДНОГ ЗНАЧАЈА

Напомена: Звездицом (*) су означени радови објављени након предходног избора у звање.

M 21

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M31

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Study of electron transmission through a platinum tube

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ABSTRACT

We have measured 200 eV electron transmission through a single platinum tube of a diameter of 3.3 mm. We find that the transmission of electrons can be detected even at large tilt angles, where the tube is not transparent geometrically. The transmission drops down exponentially with increasing the tilt angle. The energy spectrum of detected electrons behind the tube contain contributions at lower energies due to both inelastic scattering and secondary electron emission. The spectrum is qualitatively in good agreement with the calculations performed for the flat Pt surface in order to understand and model the electron interaction processes that define the transmission and the energy spectrum at the exit.

1. Introduction

There has been a large interest in recent years to investigate transmission of low-energy electrons (up to 1 keV) through nano(-micro) capillaries made of insulating materials. This investigation was triggered by the highly charge ions (HCI) *guiding* phenomenon, which was first discovered by Stolterfoht and coauthors in 2002 [1]. The HCI guiding is well explained presently and is based on the fact that the beam of charged particles dynamically deposits charge on the inner capillary surface, thus forming a Coulomb field that deflects the forthcoming particles (preventing close interaction with the surface) and efficiently guides them towards the capillary exit. A large number of papers have been published so far on this phenomenon, which offers possibilities both to study fundamental particle–surface interaction processes and to develop interesting applications such as HCI beam for nanometer-scale fabrication and MeV proton microbeams for irradiating single cells [2,3]. A comprehensive review on the subject can be found in the recent paper by Lemell et al. [4].

The first studies on electron guiding through insulating capillaries have been reported in 2007 [5,6], and followed by more detailed investigations [7–9]. The electron transmission through the capillaries appears to be fundamentally different from the simple picture of HCI guiding governed solely by Coulomb deflection [8,9]. Beside the Coulomb interaction that can also exist (although not necessary repulsive, but rather attractive due to the secondary electron emission [9]), electrons can be both elastically and inelastically scattered upon close interaction with the surface (primary projectiles) and can produce secondary electrons. Note also that electrons cannot change their charge state (in contrast to HCI), therefore it is impossible to distinguish between original and scattered projectiles. Moreover, since the dominant process upon electron transmission may be elastic electron–surface scattering, it has been suggested that even metallic (conductive) capillaries may be used for the electron guiding [8]. Following this idea, we have recently started an investigation on electron transmission through single metallic capillaries. The aim of the research is to learn about fundamental properties of both the electron guiding by metallic capillaries and the processes of electron–surface interaction that define guiding properties, as well as to investigate possible applications.

In the present paper, we report the study on the transmission of 200 eV incident electrons through a single Pt macrocapillary (3.3 mm diameter and 40.8 mm length – the aspect ratio of about 12.4). A large-diameter tube has been used, therefore the obtained results can be tested and analyzed according to the calculations made for the electron scattering by a flat Pt surface (which is more trivial), whereas the tube aspect ratio is large enough to test electron transmission at large tilt angles. The intensity of the outgoing electron current has been measured as a function of both the incident beam angle with respect to the capillary axis (the tilt angle) and the kinetic energy of outgoing electrons.

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2. Experiment

The experiment has been performed at the Institute of Physics Belgrade. The experimental system has been already described in detail elsewhere [5,7]. Additional small modifications have been made for the present study. A schematic view of the experimental setup is given in Fig. 1(a).

The system consists of an electron gun, a Pt tube attached to a 4-electrode electrostatic lens, a double cylindrical mirror analyzer (DCMA) followed by a single channel multiplier (channeltron) and a Faraday cup. Fig. 1(b) shows the realistic model of the Pt tube fitted in the 4-electrode lens, as well as electric field distributions for typically used electrode voltages, made in SIMION program [10]. Note that a penetration of the electric field inside the Pt tube, thus possible influence to electron transmission, is negligible.

The electron gun produces a well collimated electron beam with an energy spread of about 0.5 eV, which is directed into a Pt tube of 3.3 mm diameter and 40.8 mm length (the aspect ratio of about 12.4). The angle between the incident electron beam direction and the tube axis, referred as the tilt angle, can be adjusted by rotating the electron gun. At the tilt angle of 90°, the electron beam is directed into the Faraday cup, which is attached to an X–Y manipulator allowing the measuring of both the incident electron current intensity and the beam profile. The characteristic parameters of the electron beam – the diameter and the pencil angle (divergence) – are retrieved according to the simulated profile (for the identical geometry) where these parameters are adjusted to have the best fit to the experimental points. Fig. 1(c) shows a typical beam profile measured at 200 eV and the corresponding simulated curve obtained with a diameter of 0.9 mm and a divergence of 0.3°. Therefore, the incident electron beam is very well collimated and enters the Pt tube without losses.

The energy of electrons escaping the backside of the tube was analyzed using the DCMA working in a constant pass-energy mode – therefore, the count rates were recorded as a function of the retarding potential (V_R in Fig. 1(a)). It should be noted that this mode of operation provides a constant overall energy resolution, which was about 1 eV (full width at half maximum-FWHM), as measured in the elastic peak. However, the transmission of the entrance 4-electrode lens depends on the retarding potential. Therefore, the recorded kinetic electron energy distributions were corrected according to the transmission function estimated by electron ray-tracing simulations made in SIMION program [10]. The base pressure in the experimental chamber was about 7×10^{-7} mbar.

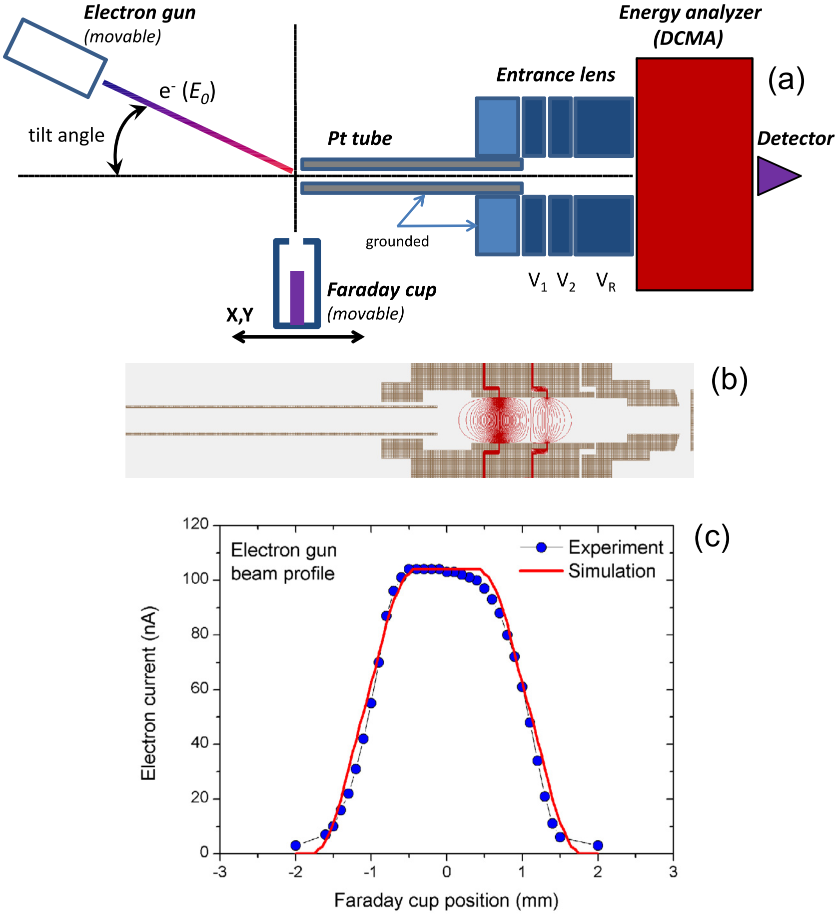

Fig. 1. (a) Experimental setup used in the present work. Electrons produced by the rotatable electron gun are directed into a Pt tube. Electrons escaping the tube are energy-analyzed. The intensity of the incident electron current and the electron beam profile are measured by using a movable Faraday cup with an entrance hole of 2 mm. (b) The realistic model of the Pt tube fitted in the 4-electrode lens made in SIMION program. The distribution of the electric field for electrode potentials typically used in the experiment are shown by red lines. (c) The 200 eV electron beam profile measured by the Faraday cup (blue circles) and the corresponding SIMION simulation (red line) obtained with the parameters: diameter = 0.9 mm; pencil angle = 0.3°. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3. Electron–surface scattering calculations

We also present calculated kinetic energy spectra of 200 eV electrons scattered from a flat Pt surface. Calculation is performed using Monte Carlo Simulation (MCS) of low energy electrons backscattered from platinum (Pt) surface [11]. In this simulation we take into account both elastic and inelastic collisions. For elastic collisions of electrons by Pt atoms, we use static field approximation with non-relativistic Schrödinger partial wave analysis [12].

For the case of inelastic scattering we use a dielectric response formalism [13–16]. According to the dielectric theory, a dielectric function $\epsilon(q,\omega)$ describes the response of a medium, as an assembly of interacting electrons and atoms, to the disturbance from an external point charge. The dielectric function $\epsilon(q,\omega)$ is the momentum (q) and energy (ω) dependent. The energy loss function $Im(-1/\epsilon(q,\omega))$, determines the probability of such an event. For the case of bulk material the energy loss function is given by the relation $Im(-1/\epsilon(q,\omega))$ and in the case of a surface it is given by the relation $Im(-1/(\epsilon(q,\omega)+1))$. For low energies, like in the present case, it is more convenient to use the surface energy loss function. The dielectric function for Pt is obtained from Refs [17,18].

We have performed MCS and calculated the backscattered electron energy loss distributions for primary and secondary electrons. Details about calculation can be found in papers [11,19] and in references there in.

4. Results and discussion

Fig. 2(a) presents a typical dependence of the detected count rate of the electrons escaping the Pt tube without an energy loss on the tilt angle. In order to avoid a saturation of the channeltron at small tilt angles, the incident current intensity was reduced to below 1 nA (such low electron currents were not measurable with the present setup). The measurements show a very narrow angular distribution of the detected electron current, which practically corresponds to the primary electron beam. Note that the aspect ratio of the Pt tube defines the maximum acceptance angle of 4.6°. Therefore, the measured angular distribution presented in Fig. 2(a) is also influenced by the electrostatic field (i.e. the focal properties of the lens – in the present case, the focus was on the elastic channel), as well as the transmission of the whole analyzer system, including the 4-element entrance lens, the double cylindrical mirror analyzer and a 3-element lens placed at the exit (see [20] for details).

Clearly, at low incident electron currents only the direct beam is detected, therefore the scattered (guided) electrons cannot be measured and studied. Still the measurements presented in Fig. 2(a) are important for the adjustment of the incident electron beam profile and the calibration of the angular scale.

In order to test a possibility of electrons being directed along the capillary axis due to the close interaction with the inner walls, as well as to measure the kinetic energy distribution of scattered electrons, the electron gun was positioned at large tilt angles and the incident electron current was increased to about 100 nA (as measured in the Faraday cup – see Fig. 1(b)). Fig. 2(b) presents a kinetic energy distribution of electrons escaping the tube at the incident energies or with small energy losses (up to about 8 eV). Clearly, the elastic peak can be detected even at very large tilt angles above the maximum value of 4.6^o as defined by the tube aspect ratio. As expected, the intensity of the transmitted (guided) electron current strongly decreases with increasing the tilt angle; the dependence is practically exponential (see the inset in Fig. 2(b)). Since the incident beam direction is far from the capillary acceptance angle, the measured signal of electrons escaping the capillary at incident energies (200 eV) must be due to the elastic electron scattering from the Pt capillary surface, thus enabling the transmission along the axis.

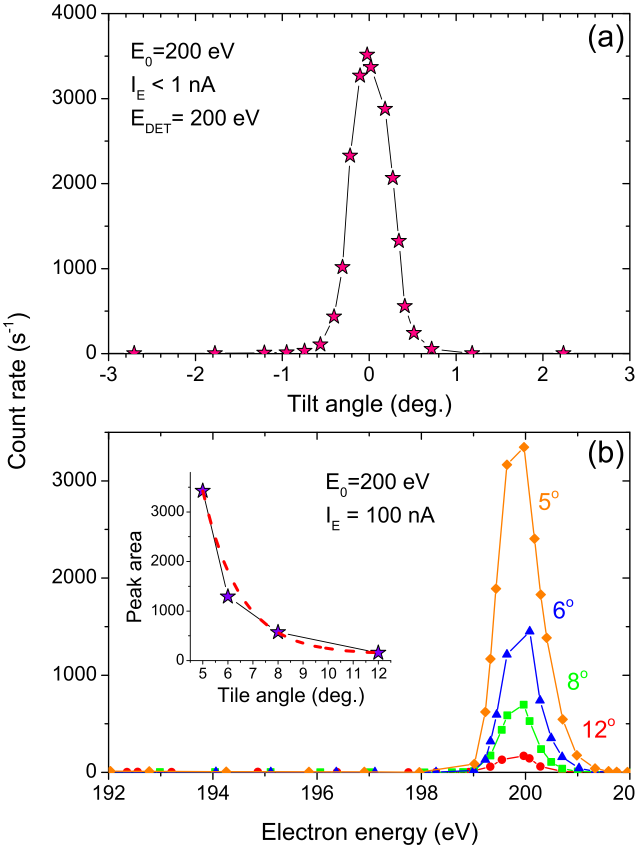

Fig. 2. (a) The intensity of the electron current escaping the Pt tube at the energy of 200 eV, as a function of the tilt angle, for the incident electron energy of 200 eV and the incident electron current intensity lower than 1 nA. (b) Experimentally obtained kinetic energy spectra of electrons escaping the Pt tube, for the incident electron energy of 200 eV, the incident electron current intensity of 100 nA and the tilt angles of 5 (diamonds), 6 (triangles), 8 (squares) and 12 (circles) degrees. The inset shows the area of the peaks presented in (b), in the energy domain from 198 to 202 eV, as a function of the tilt angle The red curve represents the exponential decay fit to the experimental points. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The close electron interaction with the inner Pt surface should also lead to both inelastic scattering and secondary electrons emission. Therefore, in contrast to the HCI guiding by insulating capillaries provided by Columbic mirror, a very broad kinetic energy distribution of escaping electrons is expected. A typical distribution obtained at the tilt angle of 6°and with the incident electron energy of 200 eV, is presented in Fig. 3(a), in a broad energy domain down to 50 eV. Apart from the sharp elastic peak that corresponds to the dominant fraction of the transmitted electrons, there is a large number of electrons at lower energies.

Fig. 3(b) shows the calculated kinetic energy distribution of electrons upon scattering of 200 eV incident electron beam from a plane Pt surface at an angle of 6°(it should be noted that the calculated distribution is not strongly dependent on the incident beam angle). The theoretical curves also separately present the yield of both the primary (due to elastic and inelastic scattering) and the secondary electrons, down to the energy of 80 eV. The experimental results are compared with the calculations by normalizing the measured curve at the energy of 185 eV. There is a good qualitative agreement between the theory and the experiment, particularly in the energy domain down to about 170 eV. Moreover, the constant increase of the secondary electrons yield as their energy decreases is also in agreement with the trend found

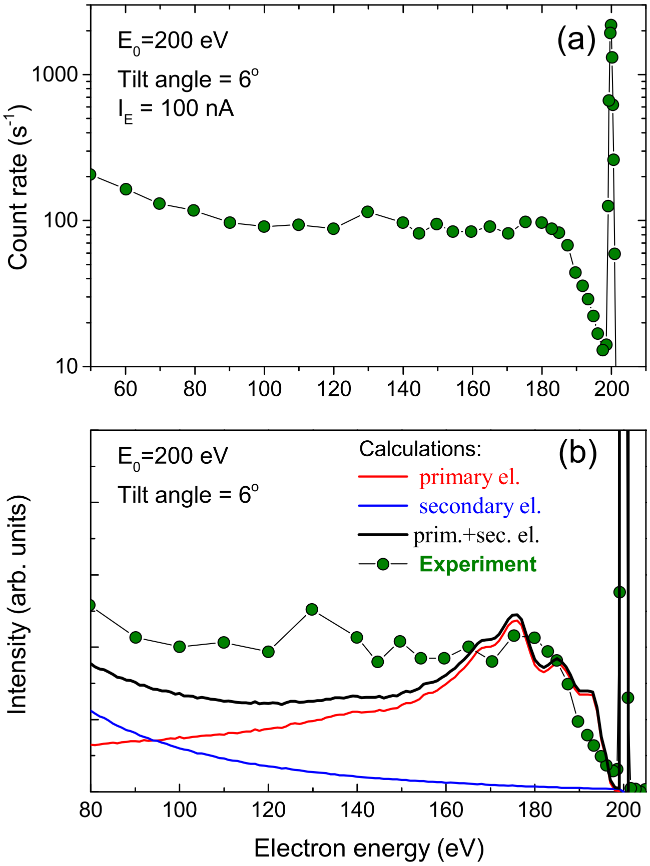

Fig. 3. (a) Experimentally obtained kinetic energy spectrum of electrons escaping the Pt tube, for the incident electron energy of 200 eV, the incident electron current intensity of 100 nA and the tilt angle 6°. (b) Calculated kinetic energy spectra of electrons scattered from a flat Pt surface, for the incident electron energy of 200 eV and the scattering angle of 6°. The experimentally obtained kinetic energy spectrum of electrons escaping the Pt tube, for the incident electron energy of 200 eV is normalized at 185 eV.

in the experiment. However, the calculated curve appears to be more structured, with pronounced shoulders, which cannot be resolved in the measured electron energy spectrum. Also, although both energy distributions are characterized by a pronounced elastic peak, the inelastic/elastic ratios are different.

The disagreement between the calculated and the measured spectra can be due to several reasons. The calculations were performed for a flat surface (to the best of our knowledge, there are no experimental results for a flat Pt surface), while in the experiment the electrons interact with the capillary surface and can suffer multiple scattering events before reaching the capillary exit and being detected. Therefore, this multiple scattering (including inelastic scattering of inelastically scattered projectiles) can smear out the respective structures seen in the theoretical spectrum. Furthermore, although the experimental spectrum has been corrected for the transmission function, the real transmission may be somewhat different from the calculated one that is based on an ideal uniform beam leaving the Pt tube and takes into account only the entrance electrostatic lens. It should be also taken into account that, in contrast to the theoretical case, the Pt surface in the experiment may be polluted from the adsorbed residual gas in the vacuum chamber. Finally, there is also an uncertainty of the calculated spectrum, dominantly because we have used a dielectric function for Pt that has been obtained by fitting the experimental results. It has been found in the present work that the calculated energy spectra were sensitive to the applied dielectric functions. However, overall, there is a good accordance between the experiment and the calculations, suggesting that the theory can be used to predict and select good candidates as materials to be used for electron transport by metallic capillaries.

5. Conclusion

In summary, we have presented a joint experimental and theoretical study on 200 eV electron transmission through a single platinum tube. We find that the transmission of electrons at their incident energies can be detected even at large tilt angles, where the tube is not transparent geometrically. The transmission drops down exponentially with increasing the tilt angle. The energy spectrum of detected electrons behind the tube contain contributions at lower energies due to both inelastic scattering and secondary electron emission. The spectrum is qualitatively in good agreement with the calculations performed for the flat Pt surface in order to understand and model the electron interaction process that define the transmission and the energy spectrum at the exit.

Although more studies with micro and nano capillaries should be performed, the present results suggest a possibility of using metallic capillaries to investigate fundamental properties of a conductive material inside a high aspect ratio pores, by use of the electron spectroscopy under ultra-high vacuum conditions. Moreover, there are potentials for interesting applications, such as the use of nano and micro high-aspect ratio metallic capillaries as a robust, spatially well-determined low-energy electron source/transporter. This could be applied, for example, to study electron driven molecular processes under different environmental conditions.

Acknowledgments

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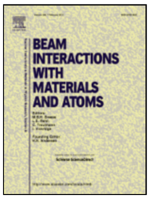

Electron transmission through a steel capillary

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ABSTRACT

The transmission of low-energy electrons through a macroscopic steel capillary has been investigated both experimentally and theoretically. The length of the steel capillary was $L = 19.5\,\text{mm}$ and the inner diameter was $d = 0.9\,\text{mm}$. The kinetic energy distribution of electrons transmitted through the steel capillary was recorded for a tilt angle of $\psi = 2.6^{\circ}$ of the incident electron beam with respect to the capillary axis. Accompanying simulations based on classical transport theory reproduce the experimental data to a high degree of agreement. Transmission for other tilt angles has also been simulated to investigate the influence of the tilt angle on the guiding efficiency.

1. Introduction

The understanding and interpretation of electron spectra backscattered from solid surfaces is important for many technical applications, e.g., for surface characterization and diagnostics to assess material damage and surface modification [1–4]. Additionally, analysis of particles scattered off solid surfaces allows for studying the scattering process itself.

With the advent of capillary targets [5,6] the change of the internal state of the (ionic) projectiles due to the close interaction with the inner capillary wall have become topics of research, since 2002 the redirection of charged particles by nanocapillary targets (see [7,8] and references therein) was investigated in detail.

In our experiment we study electrons escaping macroscopic metallic capillaries after (multiple) impact on the inner wall of the target. Deflection of incident electrons along the capillary axis is accompanied by both elastic and inelastic scattering events and the production of secondary electrons with considerable energy loss of the projectile [9–12]. Clearly, an experimental distinction between transmitted primary particles and secondary electrons generated in inelastic scattering events remains impossible and requires extensive simulations of the transmission process [13–15].

In this work we study the transmission of 150 eV electrons through a macroscopic steel capillary and model the experiment based on classical transport theory [16–19]. The theoretical spectra are presented in the energy range between 60 eV and 150 eV. For smaller electron energies calculated cross sections become unreliable.

2. Experiment

The experiment was performed on the electron spectrometer UGRA (Institute of Physics Belgrade) which has been modified to allow for mounting of a capillary target [12] instead of a gas needle. The experimental set-up is shown in Fig. 1.

The system consists of a rotatable electron gun, steel capillary, 4-electrode lens, double cylindrical mirror energy analyzer (DCMA), 3-electrode lens, channeltron as a detector and a Faraday cup for obtaining the incident electron beam profile. All components are electrically shielded and enclosed in a vacuum chamber which is magnetically shielded with two layers of μ metal. The working pressure in the experimental chamber during the measurements was about 7×10^{-7} mbar. The electron energy resolution of the system is about 0.7 eV at full width half maximum. The electron gun produces a well collimated electron beam which is directed on the capillary target.

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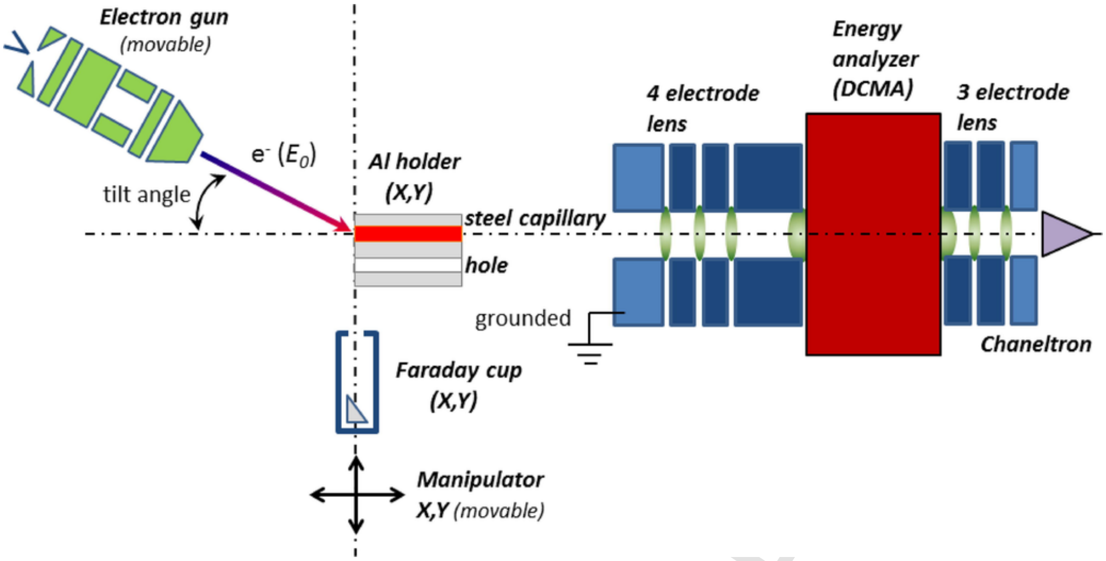

Fig. 1. The experimental set-up UGRA with the movable electron gun, stainless steel capillary, manipulator and double cylindrical mirror energy analyzer with a detector. The analyzer optics and detector are fixed in place. The X - Y manipulator is used to mount either a Faraday cup prior to experiment or an aluminum target holder with the capillary during the experiment.

To align the experimental components and to measure the electron beam profile, a Faraday cup was mounted on X - Y manipulator as indicated in Fig. 2. After optimizing and focusing the electron optics for 150 eV energy, the electron beam profile was measured by recording the current in the Faraday cup as a function of the rotation angle Θ_{relative} within the range of about ± 4° relative to the Faraday cup axis. The Faraday cup was set at a distance of 55 mm from the last electrode of the electron gun.

In order to estimate electron beam width and divergence, a SIMION simulation [20] with the real experimental electrode geometry was performed. In this simulation, starting conditions of electron trajectories were characterized by two parameters, the electron beam width w and the angular divergence da. Initial conditions were uniformly distributed within w and da. The transmission function $T(w,da)$ was simulated for different combinations of w and da until the best agreement between experimental result and simulated data was achieved (Fig. 3). From the comparison we estimated the beam divergence to be 0.3° and a beam diameter of 0.82 mm at the exit of the electron gun.

For the experiment the Faraday cup was replaced by a steel capillary with a diameter of 0.9 mm and a length of 19.5 mm. It has an aspect ratio of 21.7 or, equivalently, a geometric opening angle of 2.6°. The vertical distance between the capillary and a hole was 5.8 mm, while distance between the capillary entrance and last electron gun lens was about 25 mm. The capillary position was adjusted to align with the incident electron beam and the energy analyzer axis. The tilt angle between the incident electron beam and the capillary axis is ad-

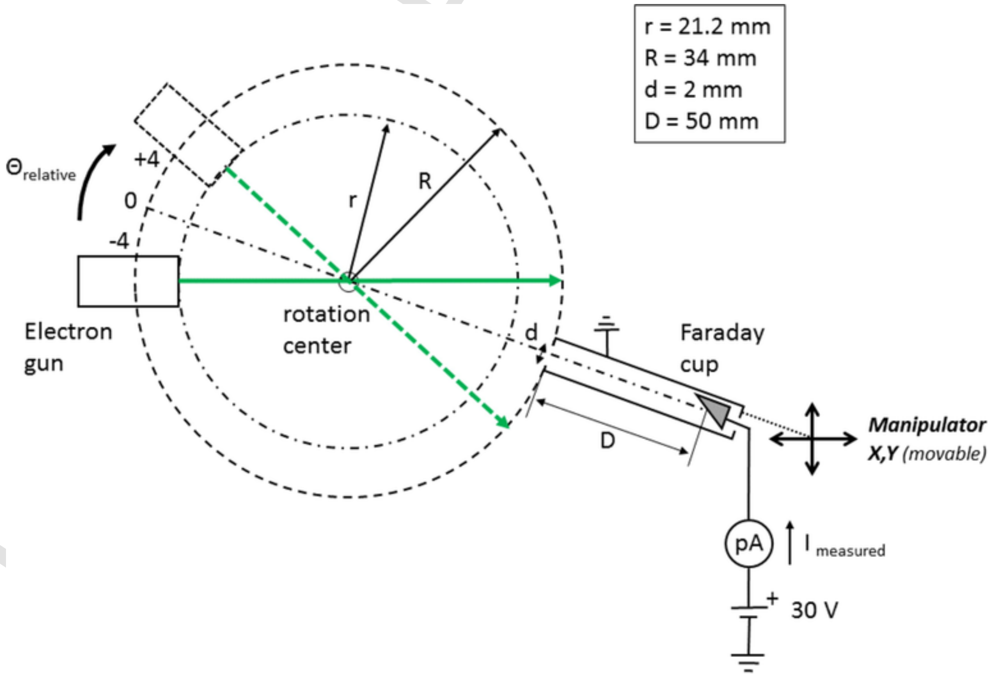

Fig. 2. Schematic representation of setup for measuring the electron beam profile.

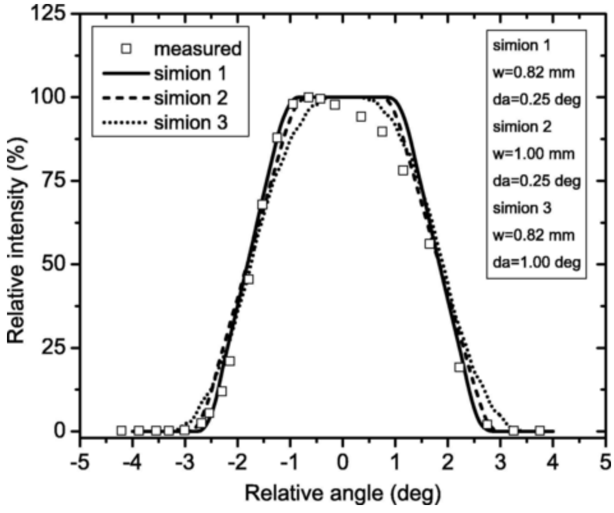

Fig. 3. Measured and simulated electron beam profiles. Symbols: measured profile, lines: SIMION simulations with different parameters; solid line – $w = 0.82$ mm, $da = 0.25°$, dash line – $w = 1.0$ mm, $da = 0.25°$, dot line - $w = 0.82$ mm, $da = 1.0°$.

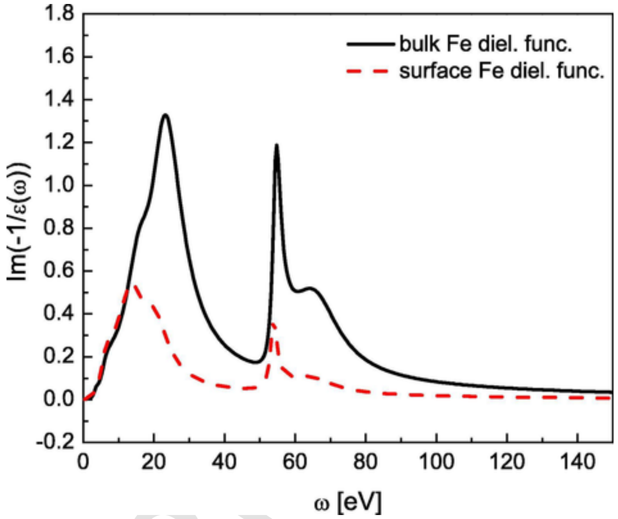

Fig. 4. Bulk (thick solid black line) and surface (thin dashed red line) dielectric functions of Fe [37]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

justed by rotating the electron gun with the capillary and analyzer remaining fixed.

The system allows for measurements of the transmitted electron current as a function of both the tilt angle and the kinetic energy of electrons escaping the capillary [12]. The electrons transmitted through the steel capillary were energy analyzed by the DCMA operating in constant pass energy mode with counts recorded as a function of a retarding potential. As the transmission of the 4-electrode lens depends on the retarding potential energy distributions of transmitted electrons were corrected according to the transmission function obtained by SIMION. An optimal system alignment was verified by measuring the total transmitted electron current at the inner cylinder of the DCMA.

3. Theory

In our simulation stainless steel is approximated with iron by neglecting any admixtures (Cr, O, C) of unknown quantity. Both elastic and inelastic collisions in Fe are taken into account. Energy dependent cross sections for elastic scattering off Fe atoms modeled with muffin-tin potential were calculated using non-relativistic Schrödinger partial wave analysis [21].

For the description of inelastic scattering cross sections we rely on the dielectric response formalism [22]. Accordingly, the momentum- and energy-loss dependent dielectric function $\epsilon(q,\omega)$ can be approximated by extrapolation of optical data $\mathrm{Im}[-\epsilon(q=0,\omega)^{-1}]$ into the q - ω plane. Then, the bulk and surface energy loss functions are given by $\mathrm{Im}[-\epsilon(q,\omega)^{-1}]$ and $\mathrm{Im}[-\{\epsilon(q,\omega)+1\}^{-1}]$, respectively [28,29]. The analytical expression given by the Lindhard [36] dielectric function provides a convenient framework for the dielectric properties of Fe. Here, surface and bulk dielectric functions were obtained following Werner et al. [37,38] (see Fig. 4).

Within the capillary electrons follow straight line trajectories. Upon impact on the inner wall of the capillary projectiles undergo a sequence of stochastic scattering events determined by the elastic and inelastic mean free paths. If an electron eventually reescapes from the inner capillary surface the next impact point on the opposite side of the capillary or its escape point from the capillary is calculated. In case of an inelastic scattering event a secondary electron is created with a kinetic energy equal to the energy lost by the primary particle. The initial direction of the secondary electron is chosen randomly from 4π. If its initial kinetic energy is larger than 60 eV its trajectory is subsequently followed as well.

4. Results and discussion

In our experiment we selected the smallest angle for which all projectiles have to interact with the inner wall of the capillary, i.e., an angle slightly larger than the geometric opening angle of the capillary. With the linear dimensions of our target capillary (diameter $d = 0.9$ mm, length $L = 19.5$ mm) the tilt angle in the experiment was set to $\psi = 2.6°$. Geometrically, the dominant fraction of electrons are expected to hit the inner surface of the capillary only once. Assuming specular reflection conditions and accounting for a beam divergence of 0.3° more than 75% are expected to undergo only one impact event, another ~20% two impact events (Fig. 5).

From the general shape of the surface and bulk dielectric loss functions (rather broad and featureless functions, Fig. 4) and the small number of impact events we expect the energy distribution of transmitted electrons to resemble the usual energy distributions after backscattering from plane solid surfaces: a sharp elastic peak together with a broad distribution of projectiles having lost a considerable fraction of their initial energy. Towards smaller energies the admixture of secondary electrons increases. Fig. 6 shows our experimental results for 150 eV electrons incident on a steel capillary under an incidence angle of 2.6° (symbols). In general, for small incidence angles one would expect the surface excitations to dominate inelastic scattering events and cause smaller energy loss. Here, however, a clear distinction between surface and bulk losses is not visible presumably due to the surface roughness of the inner wall of the capillary target accompanied by deep penetration into the target under an effectively larger incidence angle. Phonon excitations with energy losses less than about 0.1 eV will only appear as a slight broadening of the elastic peak but have not been analyzed in our experiment. The dominant loss peaks with maxima around 20 and 60 eV are the material characteristic energy losses of electrons in inelastic scattering events containing collective excitations (or plasmons) and single electron excitations. Due to the large number of d electrons in Fe the plasmon peak ($\hbar\omega_{pl} \approx 15.3$ eV) is submerged in the broad distribution around 20 eV (shoulder on the low-energy side of the distribution) and, consequently, cannot be singled out in the electron-energy spectrum as a solitary feature.

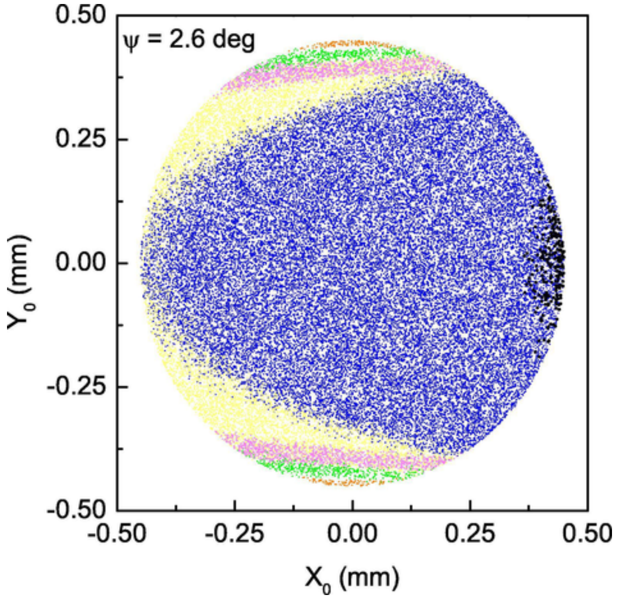

Fig. 5. Trajectories starting from randomly selected positions on the entrance plane under an incidence angle of 2.6 ± 0.3° with respect to the capillary axis are calculated assuming specular reflection upon impact on the inner capillary wall. The number of scattering events is shown in color (0: black 1: blue, 2: yellow, 3: green 4: pink, > 4: orange). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

To identify surface- or bulk-loss channels we have performed simulations allowing only for surface excitations (thin blue line in Fig. 6) and also for bulk excitations only (thick red line in Fig. 6). Neither simulation run succeeds in perfectly reproducing the experimental results. It can, however, be clearly seen that surface excitation contributions are only responsible for a small fraction of inelastic energy losses. As stated above, this points to a large surface roughness shifting the weight from surface to bulk losses. Additionally, only a minority of electrons leave the surface under the angle of incidence as assumed in the specular reflection model. Therefore, trajectories with more than one impact on the surface will feature on average a larger effective impact angle. This becomes evident when comparing Fig. 5 with Fig. 7 which shows again the starting points of trajectories on the entrance plane.

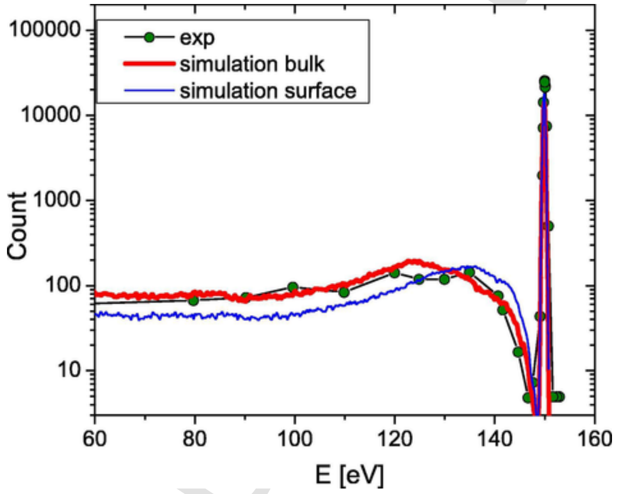

Fig. 6. Comparison between the experimentally obtained kinetic energy spectrum and calculated spectra of electrons escaping the steel tube, for an incident electron energy of 150 eV and electron beam incident angle $\psi = 2.6^{\circ}$. The simulated spectra have been obtained using the bulk dielectric function (thick red line) and the surface dielectric function (thin blue line) of iron. Experimental data are presented by green circles. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

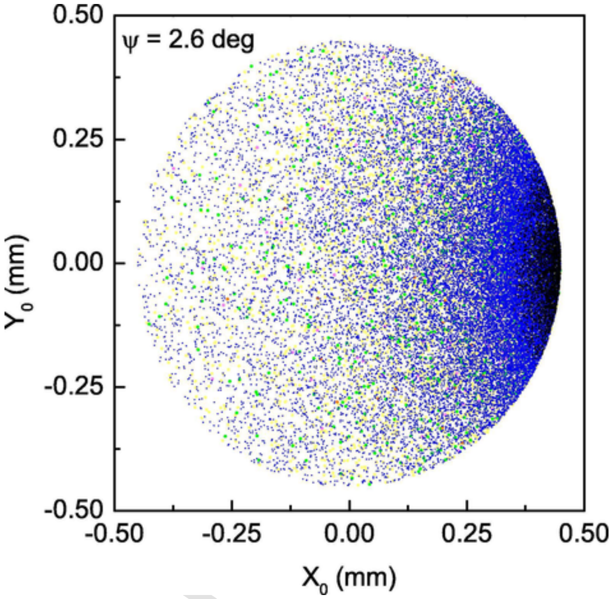

Fig. 7. Same as Fig. 5 but from results of the full simulation for an incidence angle of $\psi = 2.6 \pm 0.3^{\circ}$. (0: black 1: blue, 2: yellow, 3: green 4: pink, >4: orange). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The dominant fraction of transmitted electrons is still scattered only once but a more realistic description of the electron-wall interaction removes the boundaries between regions with different number of impact events due to an effective randomization of the exit angle from the inner capillary wall. This is also related to the neglected reflection at the collective potential of surface atoms [13] active at flat parts of the inner target wall for very grazing incidence angles. Both, the height of the elastic scattering peak in our simulation and the inelastic part of the spectrum is modeled very well.

Increasing the tilt angle in the simulations we have calculated the reduction of the transmission ratio of the capillary, i.e., number of electrons (including secondaries) divided by the number of trajectories started on the entrance plane of the capillary (Fig. 8). The energy and

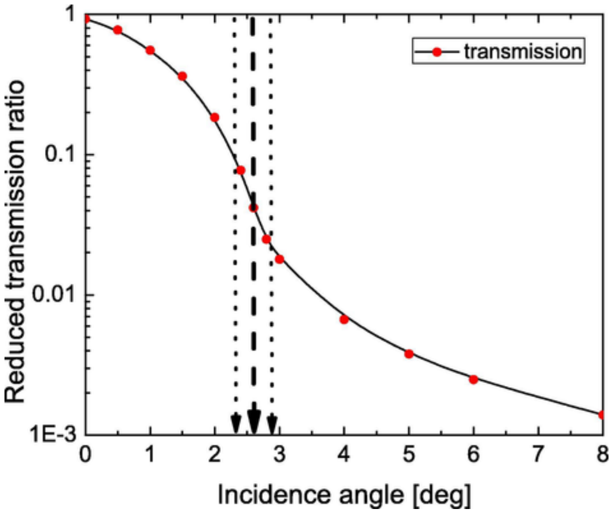

Fig. 8. Reduced transmission ratio as a function of incidence angle. The geometric opening angle is indicated by the dashed line, the beam divergence by the area between the dotted lines. Even at large incidence angles a considerable fraction of electrons are transmitted through the capillary.

incidence angle of simulated electrons were randomly picked from Gaussian distributions with $E_0 = 150$ eV, $\sigma_E = 0.5$ eV and $\sigma_\psi = 0.3^\circ$, respectively. Only electrons with kinetic energy larger than 50 eV were considered.

Two angular ranges can be discerned: as electrons hitting the surface have only a small probability to re-escape the surface the transmission ratio is for incidence angles smaller than the geometric angle dominated by transmission without interaction with the capillary wall. In contrast, for larger angles (ψ?3°) every projectiles hits the surface at least once thereby considerably reducing the transmission probability. Note, however, that even at larger angles electrons may still be transmitted at the original energy of 150 eV. In our simulation from $\psi = 2.6^\circ$ to $\psi = 5^\circ$ the total transmission probability is reduced by almost an order of magnitude (not considering the increasing intensity of low-energy electrons not included in our simulation).

5. Conclusion

We have presented a joint experimental and theoretical investigation of electrons transmission through a steel capillary with 150 eV primary incident electron energy at $\psi = 2.6^\circ$ which is tilt angle of the capillary. The electron beam divergence was 0.3°. Theoretical spectra were obtained in the energy range between 60 and 150 eV. In the simulation both elastic and inelastic scattering of primary electrons colliding with the inner capillary surface as well as secondary electron emission from the capillary wall were taken into account.

From a comparison of experimental and simulated energy spectra we conclude that the inner wall of our capillary target was very rough suppressing to a large extend specular reflection and interaction with surface loss channels. Instead, best agreement between experiment and theory was found considering only bulk excitations in the simulation of inelastic scattering processes.

Furthermore, we have calculated the transmission ratio of electrons with energies ranging from 60 to 150 eV and found a slowly decreasing transmission function outside the geometric transmission range (ψ?3°). While in specular reflection approximation projectiles would have to undergo a large number of impact events for large ψ a realistic description of the surface interaction leads to a randomization of the scattering angle and, consequently, an increased number of trajectories having suffered only few impacts.

Uncited references

[23–27,30–35].

Acknowledgments

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Dissociative electron attachment to coordination complexes of chromium: chromium(0) hexacarbonyl and benzene-chromium(0) tricarbonyl

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Full Research Paper

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Abstract

Here we report the results of dissociative electron attachment (DEA) to gas-phase chromium(0) hexacarbonyl ($Cr(CO)_6$) and benzene-chromium(0) tricarbonyl ($(\eta^6\text{-}C_6H_6)Cr(CO)_3$) in the energy range of 0–12 eV. Measurements have been performed utilizing an electron-molecular crossed beam setup. It was found that DEA to $Cr(CO)_6$ results (under the given experimental conditions) in the formation of three fragment anions, namely $[Cr(CO)_5]^-$, $[Cr(CO)_4]^-$, and $[Cr(CO)_3]^-$. The predominant reaction channel is the formation of $[Cr(CO)_5]^-$ due to the loss of one CO ligand from the transient negative ion. The $[Cr(CO)_5]^-$ channel is visible via two overlapping resonant structures appearing in the energy range below 1.5 eV with a dominant structure peaking at around 0 eV. The peak maxima of the fragments generated by the loss of two or three CO ligands are blue-shifted and the most intense peaks within the ion yield curves appear at 1.4 eV and 4.7 eV, respectively. $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ shows a very rich fragmentation pattern with decomposition leading to the formation of seven fragment anions. Three of them are generated from the cleavage of one, two or three CO ligand(s). The energy of the peak maxima of the $[(C_6H_6)Cr(CO)_2]^-$, $[(C_6H_6)Cr(CO)]^-$, and $[(C_6H_6)Cr]^-$ fragments is shifted towards higher energy with respect to the position of the respective fragments generated from $Cr(CO)_6$. This phenomenon is most likely caused by the fact that chromium–carbonyl bonds are stronger in the heteroleptic complex $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ than in homoleptic $Cr(CO)_6$. Besides, we have observed the formation of anions due to the loss of C_6H_6 and one or more CO units. Finally, we found that Cr^-, when stripped of all ligands, is generated through a high-energy resonance, peaking at 8 eV.

Introduction

Organometallic compounds are a large class of compounds with numerous applications such as homogeneous catalysts for the synthesis of fine chemicals or even enantiomerically pure products used in the pharmaceutical industry [1-3]. However, they also play an important role in nanotechnology. In fact, a number of organometallic complexes, originally designed for chemical vapor deposition (CVD) purposes, have also been recognized as promising precursors for focused electron beam induced deposition (FEBID), a process to fabricate three-dimensional metal-containing nanoscale structures [4,5]. FEBID is a direct-write technique in which a highly focused, high-energy electron beam impinges on precursor molecules physisorbed onto a substrate, thereby causing their dissociation, and in the ideal case, leading to pure deposit formation. However, the primary electron (PE) beam striking the substrate gives rise to a large amount of back-scattered electrons (BSEs) and secondary electrons (SEs) [6-8]. It is nowadays very well known that these low energy electrons (<100 eV) may induce fragmentation of the adsorbed precursor molecules via various decomposition processes such as dissociative ionization (DI), dipolar dissociation (DD), neutral dissociation (ND), and dissociative electron attachment (DEA) [8]. These reactions occur with relatively high cross sections and typically result in partial fragmentation of the precursor molecules [9-11]. Therefore, SEs may play a role in determining the composition of the FEBID deposits. Moreover, they may also be responsible for the broadening of the deposits beyond the width of the PE beam since secondary electrons create an electron flux beyond the focal area diameter of the primary beam.

To date there have been several papers devoted to the studies of the interaction of low energy electrons with gas-phase organometallic complexes. Particular attention has been paid to the compounds containing monodentate (e.g., carbonyl [12-14], trifluorophosphine [11,15], chloride [16]), bidentate (e.g., hexafluoroacetylacetone [17]), and mixed ligands (e.g., nitrosyl and carbonyl [9,10], methyl and methylcyclopentadienyl [18], π-allyl, carbonyl, bromide [19]). These studies cover both the fragmentation patterns and kinetics of electron attachment processes. It appears that for carbonyl compounds such as $Ni(CO)_4$, $Fe(CO)_5$, $W(CO)_6$, $Mo(CO)_6$, and $Cr(CO)_6$ the rate constants at thermal energy are extremely high and range from $1–3 \times 10^{-7}$ $cm^3 \cdot molecule^{-1} \cdot s^{-1}$ [13]. These values approach the maximum (s-wave) thermal attachment rate constant of 5×10^{-7} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$ at a temperature of 298 K [20].

There is, however, still a need to find more efficient FEBIP precursors that will readily detach ligands upon interaction with electrons. According to the current understanding, precursors with large organic ligands are particularly unfavorable for FEBID because they lead to codeposition of large amounts of carbon [4,21]. However, as shown in this paper, for the case of a chromium complex carrying a benzene ligand, such large organic entities may be more easy to remove by electron irradiation than generally anticipated. Chromium complexes are of interest because they are used for various technological applications [22]. For instance, Cr is used in photomasks so that Cr-containing FEBID precursors are of interest for mask repair [23] and $Cr(CO)_6$ has in fact been studied as a FEBID precursor earlier [24]. In the present work, we report the results from DEA to the gas-phase chromium(0) hexacarbonyl ($Cr(CO)_6$) and benzene-chromium(0) tricarbonyl ((η^6-C_6H_6)$Cr(CO)_3$) [25] in the energy range of 0–12 eV. The first compound is homoleptic and hence contains one type of ligand, namely CO. The other compound is heteroleptic and contains both CO and a C_6H_6 ligand. CO is a monodentate ligand which means that only one atom within the ligand binds to the central metal atom. C_6H_6 is a η^6 (hexahapto) ligand which corresponds to a contiguous series of six atoms that coordinate to the metal center. The molecular structure of both complexes is depicted in Figure 1. $Cr(CO)_6$ is a complex with 18 valence electrons (VEs) and adopts an octahedral molecular geometry, resulting in the O_h point group symmetry. Similarly, (η^6-C_6H_6)$Cr(CO)_3$ has 18 VEs. However, it has a piano stool geometry with planar arrangement of the aryl group and three carbonyl groups which act as "legs". Both complexes have spin-paired electrons and accordingly are diamagnetic. For such compounds, it has been postulated that DEA leads exclusively to the formation of fragment negative ions [26], without formation of parent anions, since the captured electron has to occupy an antibonding molecular orbital. In accordance with the predictions, we have observed the formation of three and seven fragment anions from $Cr(CO)_6$ and (η^6-C_6H_6)$Cr(CO)_3$, respectively, while the parent anion was not observed from any of the investigated complexes. In the following, the present results will be discussed in this context and in relation to the role of ligands in the respective DEA processes and compared with available literature data.

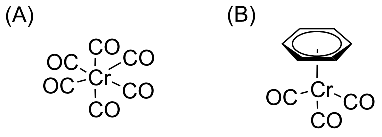

Figure 1: Structure of (A) chromium(0) hexacarbonyl and (B) benzene-chromium(0) tricarbonyl.

Experimental

Experiments were performed utilizing an electron-molecular crossed beam setup. As previously described in [27], it consists of a trochoidal electron monochromator (TEM), a quadrupole mass analyzer (QMA), and a secondary electron multiplier, which are housed in a high vacuum chamber. The electron beam (energy resolution in the range of 150–200 meV (FWHM), electron current $I \approx 10$ nA) generated with the TEM intersects with an effusive molecular beam, resulting in the formation of fragment anions. The molecular beam emanates from a vessel which was introduced directly into the oven in the vacuum chamber. In order to obtain sufficiently high vapor pressure of the target molecules in the reaction area, the oven was heated by two halogen lamps to a temperature of 90–95 °C as measured by a Pt(100) resistance mounted at one of the flanges. The generated negative ions were extracted from the reaction area by a small electric field towards the QMA entrance and detected by a single pulse counting technique. The electron energy scale was calibrated by measuring the signal of SF_6^-, exhibiting an intense resonance near 0 eV. Base pressure was in the range of 3×10^{-8} mbar while the working pressure was in the range of either $4–5 \times 10^{-7}$ mbar or $2–4 \times 10^{-5}$ mbar for $Cr(CO)_6$ and $(\eta^6\text{-}C_6H_6)Cr(CO)_3$, respectively. In spite of almost the same operative temperature for both investigated compounds, the pressure of the homoleptic compounds was substantially lower in comparison with the heteroleptic compound. This implies a lower sublimation rate for the former compound. The $Cr(CO)_6$ and $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ samples were purchased from Sigma-Aldrich with a stated purity of 98% and used as-delivered.

Results and Discussion

The impact of low-energy electrons on gas-phase chromium(0) hexacarbonyl ($Cr(CO)_6$) and benzene-chromium(0) tricarbonyl ($(\eta^6\text{-}C_6H_6)Cr(CO)_3$) has been investigated. Measurements have been taken as a function of incident electron energy in the energy range between 0–12 eV. In this energy range, it is very well known that DEA is responsible for the dissociation of the molecule. The DEA reaction is a two-step process in which, in a first step, an incident electron is captured by the target molecule to form a TNI. Since the TNI is not stable, it will decay in a second step either via autoionisation or via dissociation, forming a stable fragment anion and neutral counterpart(s). The formation of the fragment anion is only possible if the fragment at which the extra charge is localized possesses a positive value of the electron affinity. Depending on the energy at which DEA occurs, one can distinguish two types of resonances: one-particle resonance and two-particle one-hole resonance (core excited resonance) [28]. One-particle resonances take place within the subexcitation energy range <3–4 eV. They are due to a direct accommodation of the excess electrons into an unoccupied molecular orbital (MO). On the other hand, core excited resonances occur when the incoming electron transfers its energy to electronically excite the target molecule and hence becomes captured by the electron–molecule potential of the excited state.

Electron attachment to $Cr(CO)_6$ leads, under the current experimental conditions, to the formation of three anionic fragments, $[Cr(CO)_5]^-$, $[Cr(CO)_4]^-$, and $[Cr(CO)_3]^-$. The ion yield curves of these fragments are shown in Figure 2. The corresponding fragment anions are generated via:

$$e^- + Cr(CO)_6 \rightarrow \left[Cr(CO)_6\right]^{\#-} \rightarrow \left[Cr(CO)_5\right]^- + CO \quad (1)$$

$$\rightarrow \left[Cr(CO)_4\right]^- + 2CO \quad (2)$$

$$\rightarrow \left[Cr(CO)_3\right]^- + 3CO \quad (3)$$

The predominant reaction channel is the formation of $[Cr(CO)_5]^-$ through the cleavage of one CO ligand from the transient negative ion. This fragment shows a narrow and intense structure close to 0 eV within the ion yield curve and a less intense peak at 1 eV, which are attributed to one-particle resonances. The positions of the peaks correlate very well with the positions of the resonances reported from electron transmission spectroscopy (ETS) experiments [29]. Indeed, from ETS, the features emerge below 1 eV implying the occurrence of an attachment of electrons with energy close to 0 eV and near 1 eV. Based on the calculations, it has been suggested that the low energy maximum can be attributed to a negative ion state

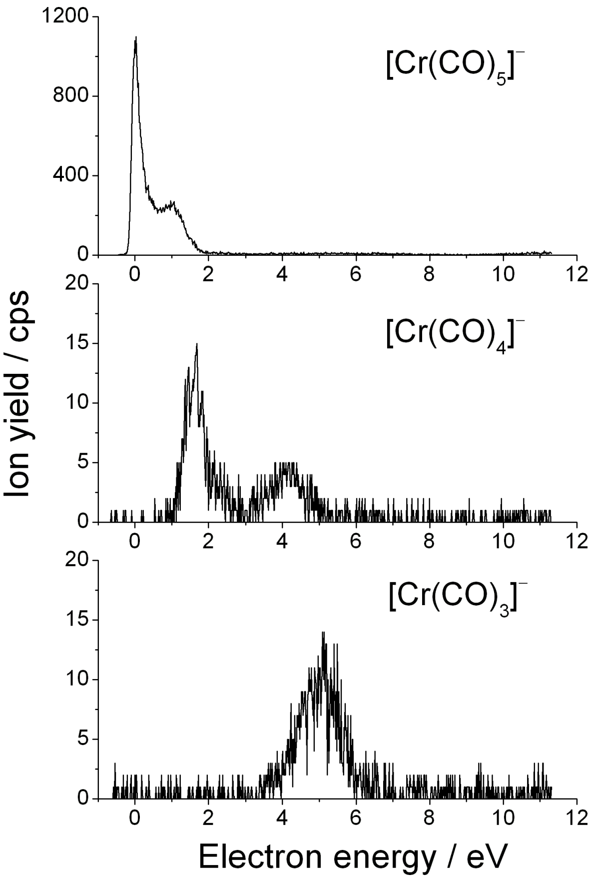

Figure 2: Yield of the fragment anions generated from DEA to chromium(0) hexacarbonyl.

emerging from electron capture into the $3t_{2g}$ orbital of this molecule [30]. A high cross section for the $[Cr(CO)_5]^-$ ion formation already at energy close to 0 eV implies that the reaction is most likely exothermic, i.e., the electron affinity of the $Cr(CO)_5$ fragment exceeds the bond energy of Cr−CO. According to the literature, the bond dissociation enthalpy of $Cr(CO)_5$−CO is equal to 1.6 eV [31], therefore the electron affinity of $Cr(CO)_5$ should be ≥1.6 eV. A further reaction channel in DEA to $Cr(CO)_6$ is the formation of $[Cr(CO)_4]^-$, formed from the loss of two CO ligands. The ion yield curve is composed of two peaks, centered at 1.4 eV and 4.1 eV. The position of the first peak correlates well with the position of the resonance observed from ETS studies that has been assigned to capture into the $3t_{2u}$ orbital of this molecule [30]. Further abstraction of the CO ligand leads to the formation of $[Cr(CO)_3]^-$ which extends from 3.3 to 6 eV and peaks at 5.0 eV. This structure can be attributed to a core excited resonance, however it should be stressed here that one-particle resonances may also be formed in this energy range and cannot be ruled out.

DEA studies on $Cr(CO)_6$ have already been reported by Tossell et al. [30] as well as Winters and Kiser [32]. In the former paper, the negative ion current from $Cr(CO)_6$ as a function of incident electron energy has been shown. The reported dominant feature was observed near 0.5 eV with shoulders between 1 and 2 eV and between 2 and 3 eV, which is in a fairly good agreement with our experimental results. The authors concluded that the vast majority of the ions observed were $[Cr(CO)_5]^-$. The only exception was a peak near 1.6 eV where $[Cr(CO)_4]^-$ contributed about 15% to the total ion current. In contrast, Winters and Kiser have observed formation of six fragment anions, i.e., $[Cr(CO)_5]^-$, $[Cr(CO)_4]^-$, $[Cr(CO)_3]^-$, $[Cr(CO)_2]^-$, $[Cr(CO)]^-$, and $[Cr]^-$ [32]. In analogy to our results, the most intense fragment was generated from the cleavages of single CO ligands. The $[Cr(CO)_4]^-$ and $[Cr(CO)_3]^-$ anions were generated with an intensity of 30% of the main signal. Further signals were observed with relative intensity of 10%, 5%, and <5% for $[Cr(CO)_2]^-$, $[Cr(CO)]^-$, and $[Cr]^-$, respectively. Hence, the intensity of the missing fragments in our experiment is below the detection limit of our experimental setup. In particular, if we take into account that the intensity of the $[Cr]^-$ signal in Winters and Kiser's experiment is lower than 5% of $[Cr(CO)_5]^-$ at 2.4 eV, we end up at the noise level. However, in their studies, Winters and Kiser could only observe a single peak for any of the reported fragment anions appearing above 2 eV. It should be stressed here that the maximum of the second peak for $[Cr(CO)_4]^-$ and the maximum of the peak for $[Cr(CO)_3]^-$ observed within the present studies match reasonably well to the position of the peaks reported by Winters and Kiser. There is, however, a big discrepancy between the positions of the dominant $[Cr(CO)_5]^-$ fragment. While in our studies the main peak appears already near 0 eV with a contribution at 1 eV, from the experiment of Winters and Kiser, it is reported to peak at 2.4 eV. It should be emphasized that the appearance of all observed anions, including the main peak of the $[Cr(CO)_5]^-$ ion, above 2 eV in the latter studies contradicts also with the results of George and Beauchamp, who have shown that the rate constants at the thermal energy for dissociative electron capture by $Cr(CO)_6$ approach the maximum thermal attachment rate constant equals to 3.2×10^{-7} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$ [13].

A particularly extensive fragmentation has been observed in DEA to the heteroleptic complex $(\eta^6\text{-}C_6H_6)Cr(CO)_3$. In the case of electron attachment to $(\eta^6\text{-}C_6H_6)Cr(CO)_3$, we observe the production of seven fragment anions: $[(C_6H_6)Cr(CO)_2]^-$, $[(C_6H_6)Cr(CO)]^-$, $[(C_6H_6)Cr]^-$, $[Cr(CO)_3]^-$, $[Cr(CO)_2]^-$, $[CrCO]^-$, and Cr^- in the electron energy range of 0–12 eV. These fragments can be divided into two groups: a first group which contains the anions generated by the loss of one or more CO ligands and the second one which includes the anions formed from the loss of the C_6H_6 unit or the loss of C_6H_6 and one or more CO units. The fragment anions which form the first group are generated via:

$$e^- + (C_6H_6)Cr(CO)_3 \rightarrow \left[(C_6H_6)Cr(CO)_3\right]^{\#-} \rightarrow \left[(C_6H_6)Cr(CO)_2\right]^- + CO \quad (4)$$

$$\rightarrow \left[(C_6H_6)CrCO\right]^- + 2CO \quad (5)$$

$$\rightarrow \left[(C_6H_6)Cr\right]^- + 3CO \quad (6)$$

The ion yield curves of these fragments are shown in Figure 3. At first glance it becomes obvious that the predominant fragment is due to the loss of one CO ligand. This is consistent with our results obtained for the homoleptic chromium complex $Cr(CO)_6$ as well as the previously studied ruthenium complex containing multicoordinated π-allyl ligands $(\eta^3\text{-}C_3H_5)Ru(CO)_3Br$ [19]. The $[(C_6H_6)Cr(CO)_2]^-$ anion is visible via two strongly overlapping structures at 0.85 eV and 1.7 eV. Hence, it is shifted towards higher energy with respect to the position of the fragment anion formed from the loss of a single CO ligand from $Cr(CO)_6$. This shift can be caused mainly by the fact that chromium–carbonyl bonds are stronger in the heteroleptic complex $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ than in homoleptic $Cr(CO)_6$ (see [31] and references therein). The $[(C_6H_6)CrCO]^-$ channel associated with the loss of two CO groups has a threshold at 2.5 eV and two resonances are present within the yield curve peaking at 3.5 eV and 8.3 eV. The abstraction of a further CO unit results in the formation of $[(C_6H_6)Cr]^-$. The threshold for this reaction channel is somewhat shifted towards higher energy, that is to 3.3 eV, in comparison to the fragment formed from the loss of two CO units. Within the ion yield curve one can distinguish three resonances centered at 4.1, 6.0 and 8.2 eV. From Figure 3 it can be clearly seen that the efficiency of the reaction channel decreases with the number of carbonyl groups that are detached from the TNI to form the respective anions. This behavior has already been reported from DEA to metal carbonyls (e.g., $Ni(CO)_4$, $Fe(CO)_5$, $Cr(CO)_6$, $Mo(CO)_6$, $W(CO)_6$) [32], as well as from cobalt tricarbonylnitrosyl [9], and π-allyl ruthenium tricarbonyl bromide [19].

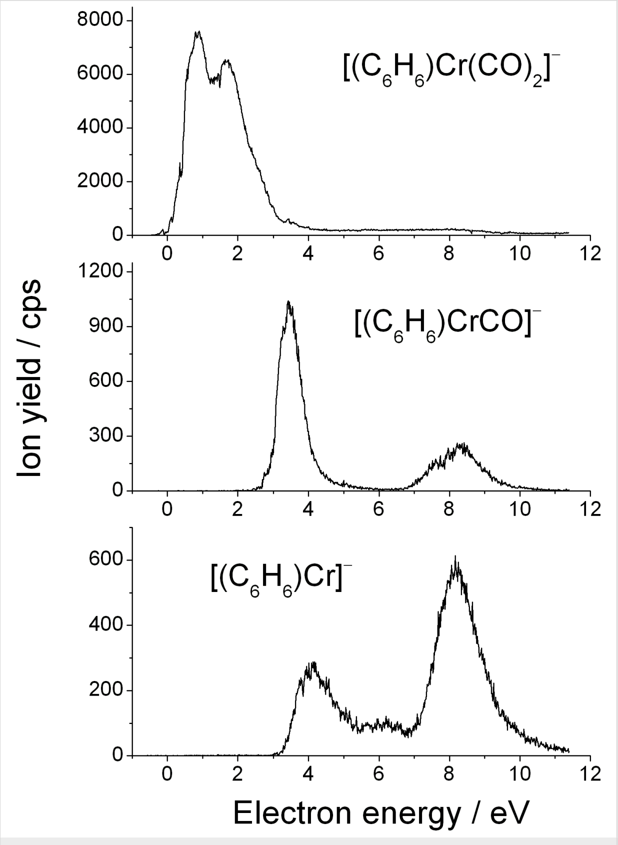

Figure 3: Yield of the fragment anions $[(C_6H_6)Cr(CO)_2]^-$, $[(C_6H_6)Cr(CO)]^-$, and $[(C_6H_6)Cr]^-$ obtained from DEA to benzene-chromium(0) tricarbonyl which are generated by the loss of one, two, and three carbonyl groups, respectively.

The second group of anionic products is formed by the following four dissociative channels:

$$e^- + (C_6H_6)Cr(CO)_3 \rightarrow \left[(C_6H_6)Cr(CO)_3\right]^{\#-} \rightarrow \left[Cr(CO)_3\right]^- + C_6H_6 \tag{7}$$

$$\rightarrow \left[Cr(CO)_2\right]^- + C_6H_6 + CO \tag{8}$$

$$\rightarrow \left[CrCO\right]^- + C_6H_6 + 2CO \tag{9}$$

$$\rightarrow \left[Cr\right]^- + C_6H_6 + 3CO \tag{10}$$

As mentioned above, this group consists of fragment anions generated from the loss of the C_6H_6 ligand or the loss of C_6H_6 and one or more CO ligands to form $[Cr(CO)_3]^-$, $[Cr(CO)_2]^-$, $[CrCO]^-$, and Cr^-, respectively (Figure 4). The predominant

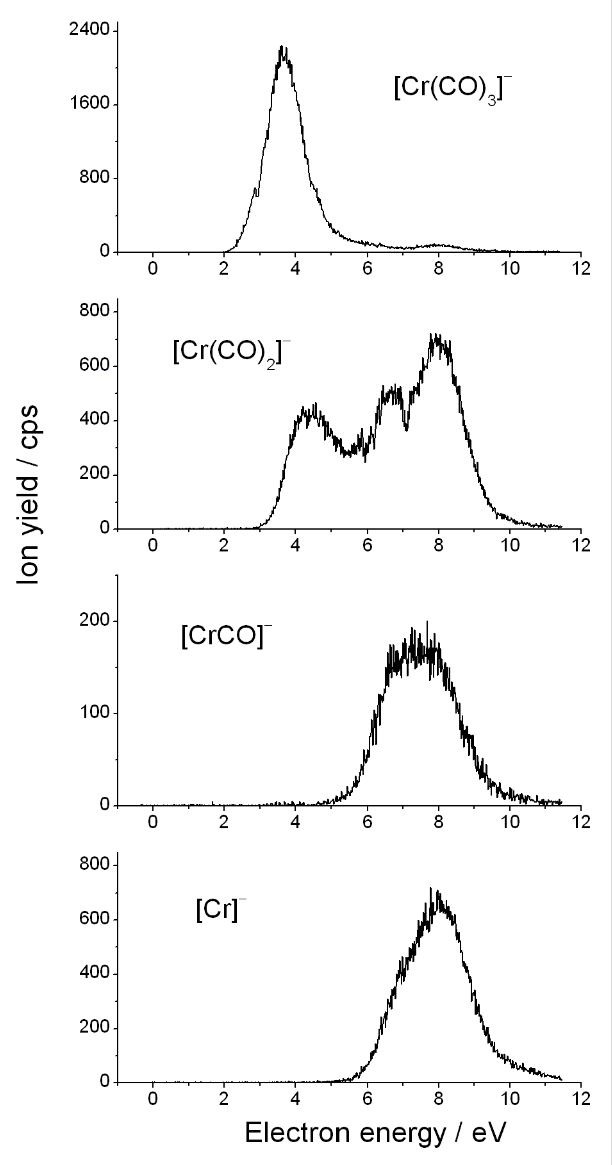

Figure 4: Yield of the fragment anions $[Cr(CO)_3]^-$, $[Cr(CO)_2]^-$, $[CrCO]^-$, and Cr^- obtained from DEA to benzene-chromium(0) tricarbonyl.

fragment from the second group is formed as a result of the loss of the C_6H_6 unit. The main contribution to the ion yield of $[Cr(CO)_3]^-$ is visible through a resonance structure peaking at 3.7 eV with a low intensity structure at around 7.9 eV. Considering all the fragments generated from DEA to $(C_6H_6)Cr(CO)_3$, this is the second most intense signal. Such a high intensity of $[Cr(CO)_3]^-$ has to be related to the lability of the C_6H_6 group. This is a striking finding since, in general, the multicentered π-bonded ligands are recognized to be particularly persistent in FEBID, and hence should be avoided [18,19]. However, it should be emphasized here that the C_6H_6 group is neutral in contrast to, for example, the methylcyclopentadienyl ligand, which may facilitate the detachment of the C_6H_6 group from the $(C_6H_6)Cr(CO)_3$ complex.

The $[Cr(CO)_2]^-$ anion extends in a very broad energy range from 3.3 eV to 10 eV and is visible via three strongly overlapping resonant structures peaking at 4.5, 6.5 and 7.9 eV. Further loss of CO results in the formation of $[CrCO]^-$ which appears in the high energy domain with a peak maximum at 7.5 eV. Since the peak is very broad, the threshold for the reaction channel is as low as 5.5 eV. Finally, we would like to point out that we observe the formation of a bare chromium anion, Cr^-. The yield curve of Cr^- stretches from 6 to 11 eV and peaks around 8 eV and has a pronounced shoulder at the low energy side. It is worth mentioning that Cr^- is generated with an exceptionally high relative cross section, which is untypical when considering organometallic complexes including those with multicoordinated ligands. Indeed, as obvious from the reports on $(\eta^3\text{-}C_3H_5)Ru(CO)_3Br$ [19], $MeCpPtMe_3$[18], $Co(CO)_3NO$ [9], and $HFeCo_3(CO)_{12}$ [33], the bare metal ions were either not observed or observed with very low intensity (below 0.5% of the most intense anionic fragment).

Conclusion

In the present contribution, we have investigated how different ligands within coordination complexes modify the formation of transient negative ion (TNIs) and their subsequent decay by dissociation. In particular, by selecting homo- and heteroleptic complexes, namely $Cr(CO)_6$ and $(\eta^6\text{-}C_6H_6)Cr(CO)_3$, we have studied the influence of the substitution of three CO units by the hexahapto C_6H_6 unit on electron-induced fragmentation. In general, we have observed the electron-driven decomposition of chromium(0) hexacarbonyland benzene-chromium(0) tricarbonyl complexes into three ($[Cr(CO)_5]^-$, $[Cr(CO)_4]^-$, and $[Cr(CO)_3]^-$) and seven ($[(C_6H_6)Cr(CO)_2]^-$, $[(C_6H_6)Cr(CO)]^-$, $[(C_6H_6)Cr]^-$, $[Cr(CO)_3]^-$, $[Cr(CO)_2]^-$, $[CrCO]^-$, and Cr^-) fragment anions, respectively. The energy of the peak maxima and intensity of the $[M\text{–}(CO)_x]^-$ fragment anions (where M = neutral molecule, and x can be equal to 1, 2 or 3) generated from both investigated complexes varied in an anticipated fashion. Such a stepwise increase in the energy and decrease in the intensity as more CO ligands are removed has been previously reported for a series of transition-metal carbonyls [14,32]. It has also been suggested that such a behavior may be reminiscent of a successive removal of CO fragments in the cracking patterns of the negative ions. Hence, it is very likely that the $[M(CO)_x]^-$ anions, besides the direct decomposition of TNI, may also be generated via sequential, metastable decay.

In the framework of the potential role of coordination complexes of chromium for FEBID applications, we note that the removal of C_6H_6 and all CO ligands to form exceptionally intense signal of bare $[Cr]^-$ has been observed in DEA to $(\eta^6\text{-}C_6H_6)Cr(CO)_3$. On the basis of our results it seems to be plausible to consider a multicentered benzyl group as a promising leaving group within FEBID precursors.

Acknowledgments

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Regular Article

Elastic electron scattering cross sections for triethyl phosphate molecule at intermediate electron energies from 50 eV to 250 eV[⋆,⋆⋆]

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Abstract. We present a combined experimental and theoretical study of the electron elastic differential cross sections of triethyl phosphate molecule $(C_2H_5)_3PO_4$ (TEP). The experimental setup based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron was used to measure differential cross sections. The absolute scale for the cross sections is obtained by relative-flow method using argon gas as a reference. For the interpretation of the measured data we applied the partial expansion method to calculate the elastic cross sections of TEP. We found excellent agreement between the shapes of measured and calculated data.

1 Introduction

Electron interaction research with biological material, as well as subsequent damage caused by in the media, has attracted a considerable scientific interest in recent years, especially in molecular physics and biomedicine. The reason for this is the fact that electrons play a key role in numerous biomedical applications, for both diagnostic and therapeutic purposes. Today it is well accepted that secondary electrons (SE) are extensively generated by passing primary beam through the medium ($\sim 4 \times 10^4$ per MeV energy transferred to the medium) and are considered the main cause of radiation damage in biological tissues [1].

Due to a large number of involved processes, the mechanism of damaging of a complex DNA by the radiation molecule is very difficult to clarify. Studies with isolated DNA elements (e.g. nucleobases [2]) or with molecules analogous to DNA (e.g. molecules analogous to deoxyribose [3–6] or molecule analogous to pyrimidine bases [7]) provide a good insight into the molecular mechanisms that lead to the DNA damage, which connects the macroscopic effects of radiation with molecular-level damage.

The motivation to study electron interaction with triethyl phosphate (TEP, $C_6H_{15}O_4P$) comes from radiation damage research, since this molecule may be considered as an analogue to phosphate group, which together with the sugar deoxyribose, forms the backbone of the DNA molecule (see Fig. 1). Our results should bring information about electron–triethyl phosphate interactions and we will discuss their relevance to electron-induced damage to the DNA backbone. This investigation also would be an extension to our previous measurements with molecules that are analogue to some parts of DNA molecule [3–7]. To our knowledge, there are no published absolute differential cross sections for electron interaction by triethyl phosphate in this intermediate electron energy range.

Dissociative electron attachment spectrum for TEP and for low energy incident electrons has been reported [8]. In that research authors used triethyl phosphate molecule to simulate the behavior of the phosphate group in DNA towards the attack of low energy electrons. They found that the compound undergoes effective dissociative electron attachment within a low energy resonant feature at 1 eV and a further resonance peaking at 8 eV [8]. Also

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[⋆] Contribution to the Topical Issue "Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces", edited by Károly Tőkési, Béla Paripás, Gábor Pszota, and Andrey V. Solov'yov.

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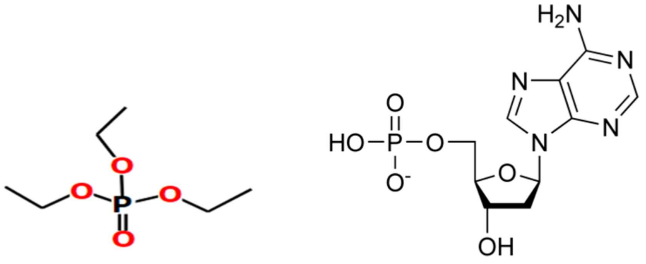

Fig. 1. Triethyl phosphate (TEP) and DNA backbone.

investigating DEA processes on TEP [9] it has been found the loss of an ethoxy radical due to P–O bond cleavage. It was emphasized that for the phosphate group in DNA both reactions would correspond to a direct single strand break [9].

In this paper, absolute differential cross sections (DCSs) for elastic electron-TEP scattering at incident electron energies from 50 eV to 250 eV are presented. Results are obtained using crossed electron-target beam apparatus. Absolute values, which are used to normalize relative DCSs, are determined by the relative flow method.

2 Experiment

The experimental results are obtained on the crossed electron-atom (molecule) beam apparatus. Incident electrons are derived from an electron gun that consists of seven electrodes; four for the extraction of electrons emitted by thermoelectronic emission from the cathode and three for the focusing of the beam to the interaction volume. The electron energy is determined by the potential difference between the cathode and the last electrode which is grounded and can be varied in the range from 40 eV to 300 eV. Energy resolution of the electron spectrometer is defined by the thermal distribution of the primary electrons and is approximately 0.5 eV.

The electrons interact with a molecular beam formed by a stainless-steel gas needle and further slowed down and focused by the four-element electron lens into the double cylindrical mirror analyzer which selects them by the energy. After passing through the analyzer, the electrons are focused by three-element electron lens to the detector, single channel electron multiplier. All mentioned experimental elements are located inside a vacuum chamber. Base pressure of about 6×10^{-7} mbar, is achieved using a turbo molecular pump. The operating pressure was about one order higher. The electron gun can be rotated around the gas needle from $-40°$ to $130°$, while the angular resolution of the analyzer was approximately $\pm 2°$.

The relative DCSs for elastic electron scattering are measured as a function of scattering angle, from 25° to 125° (in 5° steps), at a given electron impact energy from 50 eV to 250 eV (in 50 eV steps). The intensity of elastically scattered electrons is measured at the maximum of elastic peak in energy loss spectrum and is directly proportional to the relative DCSs at a selected electron energy. In this experiment, voltages on electron gun and double cylindrical mirror analyzer are adjusted so that the scattering volume is within the view cone of the analyzer, achieving the interaction volume constant. The deviations can occur at small scattering angles (below 35°). Corrections at the small angles and lower energies are made by comparing the cross sections for noble gases, in this case argon, with previous published results from other authors. The contribution of background is measured by introducing target gas into the chamber through the side leak (it has been around 10–15% of the true signal) and is subtracted from the apparent signal for each measured point. These two measurements were performed at least three times for each electron energy of interest. Subtracting the background from signal yields three corrected measurements which were weighted and averaged. For each electron energy, the analyser was set to allow the electrons corresponding to the elastic peak to pass through. Accordingly, the electron gun and two lenses before and after the analyser were readjusted for optimal signal and to compensate for the transmission functions.

The relative differential cross-sections are further normalized to the absolute scale using absolute points (at the angles 40°, 80°, 90° or 100°), by the relative flow method. Argon was used as the referent gas, with known cross sections published by Ranković et al. [10] for the incident electron energies from 50 eV to 200 eV, and Williams and Willis [11] for electron energy 250 eV. In this method, the signal of the elastic scattered electrons for the target molecule is compared with the signal for the referent gas, at the same angle of scattering, for the same energy of the incident electrons, under the same experimental conditions. In order to provide the same experimental conditions (the same profiles of the beams, the same mean free paths [12], the pressure ratio behind the gas needle of the tested molecule and the reference gas must be inversely proportional to the ratio of the squares gas kinetic diameters. Since it is known that the gas kinetic diameter of argon is 3.58 Å, and for triethyl phosphate it is taken to be approximately 8 Å, then the necessary pressure ratio is set at about 5. The relative flow rate has been determined by closing an outlet to the chamber, admitting target gases into a closed constant volume and then measuring the pressure increase in time (measured by a MKS baratron). The flow is determined from the experimental curve of pressure versus time fitted by the least-squares method. The background contribution for each measured point, which contains both argon and triethyl phosphate, is subtracted from the signal. The influence of adsorption effects on gas line surfaces to the relative flow measurements [13] is reduced in the present case by heating the whole system.

TEP was purchased from Aldrich with a declared purity better than 99%. Before starting the measurements a few freeze-thaw-pump cycles under vacuum have been made. TEP is a liquid at room temperature and was introduced into the scattering region from a glass container via gas line system. This molecule is characterized by low vapor pressure (0.39 mmHg at 25°C) and very high dipole moment (2.86 D). Therefore, for stable experimental conditions during gas phase measurements, target container was heated around 80°C, like for previously studied "sticky" molecular targets such as THF and its

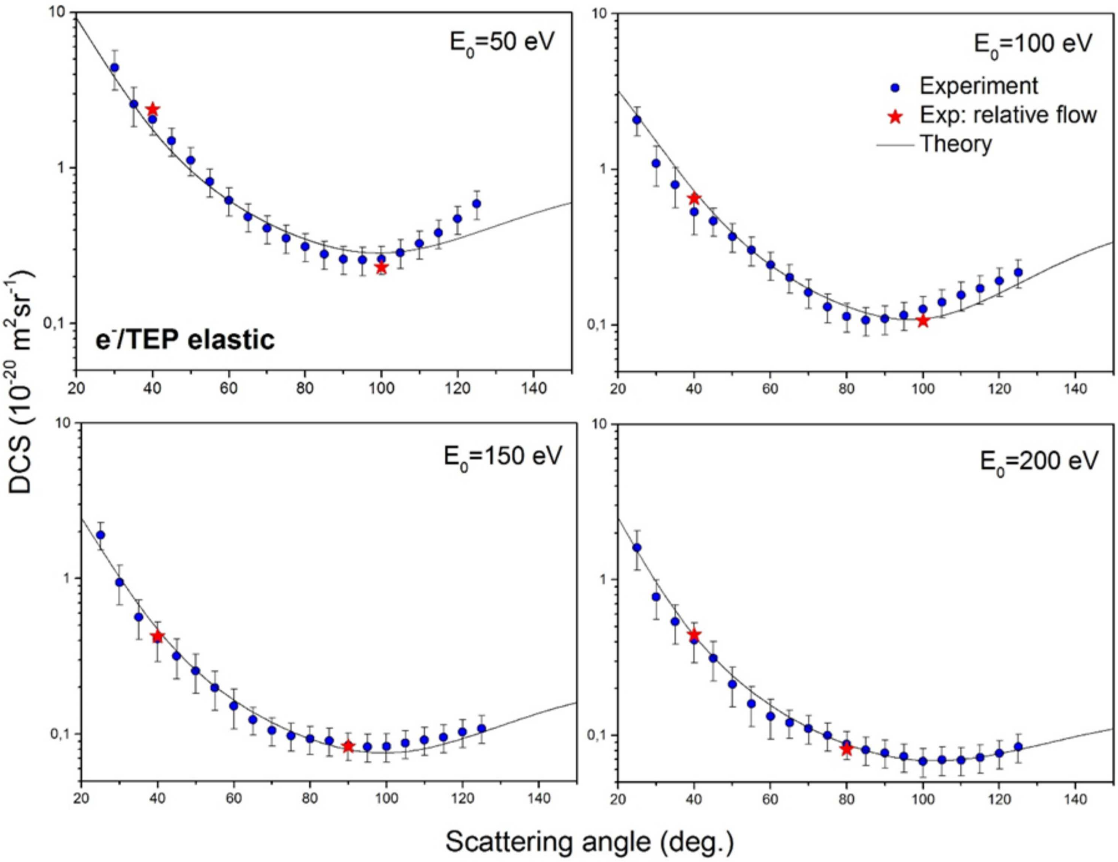

Fig. 2. Angular dependence of the DCSs for elastic electron scattering from TEP at different, fixed incident energies. Circles represent absolute experimental differential cross sections; stars represent absolute values obtained by relative flow method, where reference points for Ar are taken from paper by Ranković et al. [10]; full line represents theoretical results. Theory is normalized to the experimental results.

derivatives [14]. In the present work, pipes and the needle were also heated providing a stable driving pressure behind the needle and also for avoiding the absorption effects.

The errors of the relative cross section include statistical errors (0.2–4%) and errors due to the instability of the system, short term stability errors, which are determined by the spread in the repeated measurements at the same electron energies and the same scattering angle (1.5–6%). The total error of relative measurements was increased by 20% at small scattering angles due to the possible change in the interaction volume. The errors for absolute differential cross sections are dominated by the errors of the reference DCSs for Ar. Errors for the flow rate are ignored due to stable experimental conditions and linear pressure increase with time. The errors for the reference absolute DCSs are about 20%. The total errors for absolute DCSs are about 25%.

3 Theory

In this work, the key of the determination of the elastic cross section calculations of TEP is the atomic cross section calculations for the components of the molecule. The calculated atomic cross sections were simple added according to the stoichiometry numbers to estimate the elastic cross section of TEP. We note that in this way maybe the absolute cross sections of the molecule are overestimated because the shielding of the cross sections for various component of the molecule is not taken into account. However, we believe that the shape of the angular differential cross can be calculated accurately.

For the atomic target the partial expansion method was used to describe the differential cross sections for elastic scattering. The relativistic differential cross section per unit solid angle is given by the following form:

$$\frac{d\sigma_e}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2, \tag{1}$$

where θ is scattering angle, $f(\theta)$ and $g(\theta)$ are the spin-up and spin-down scattering amplitudes. $f(\theta)$ and $g(\theta)$ can be expressed as:

$$f(\theta) = \sum_{l=0}^{\infty} F_l P_l(\cos(\theta)), \tag{2}$$

$$g(\theta) = \sum_{l=0}^{\infty} G_l P_l^1(\cos(\theta)), \tag{3}$$

where $P_l(\cos(\theta))$ are the Legendre polynomials, $P_l{}^1(\cos(\theta))$ are the associated Legendre functions. F_l and G_l can be calculated according to following relations:

$$F_l = \frac{1}{2ik}\left\{(l+1)\left[\exp\left(2i\delta_{l+}\right)-1\right]+l\left[\exp\left(-2i\delta_{l-}\right)-1\right]\right\} \tag{4}$$

$$G_l = \frac{1}{2ik}\left[\exp\left(2i\delta_{l-}\right)-\exp\left(-2i\delta_{l+}\right)\right] \tag{5}$$

where δ_{l+}, δ_{l-} are the phase shift of the order l, and k is the momentum of the projectile electron. Details of the calculations can be found in reference [15].

4 Results

Absolute differential cross sections for elastic electron scattering from TEP molecule are presented in Figure 2. (circles-measured points; full line-calculated values) for the incident electron energies from 50 eV to 250 eV. Absolute DCSs for Ar in the energy range from 50 eV to 200 eV are taken from Ranković et al. [10]. In Figure 3. absolute differential cross sections for the incident electron energy of 250 eV are presented, where referent absolute cross sections for Ar are taken from the paper Williams and Willis [11]. Absolute points obtained by the relative flow method, on certain incident electron energies and scattering angles, used for normalization of relative measurements on absolute scale, are presented as well (stars). It can be noted that the absolute points agree well with the independently measured relative differential cross sections, which can be used as confirmation of the reliability of experimental methods, because it comprises of two independent set of data. The measured absolute results are also shown in Table 1. Theoretical results are normalized on the experimental data at an angle of 60°, for the incident electron energies 50 eV, 100 eV and 250 eV, and 80° for energies 150 and 200 eV. The agreement between the measured points and the theory is within the experimental error in the whole angular range, except for energy 50 eV at larger scattering angles, where the experimental results are slightly higher on the absolute scale. DCSs show a wide minimum at the scattering angle about 90°, for the energies 50 eV and 100 eV, which slowly disappears for energies above 150 eV. This tendency is also observed in DCSs for elastic electron scattering on other previously measured molecules [3–7]. This indicates a similar redistribution of elastically scattered electrons on molecules analogous to the DNA building blocks in the medium energy range. In the investigated energy range, from 50 eV to 250 eV. Absolute differential cross-sections are reduced by about an order of magnitude, in the energy range from 50 eV to 250 eV. That behavior we have also noticed for previous targets [3–7].

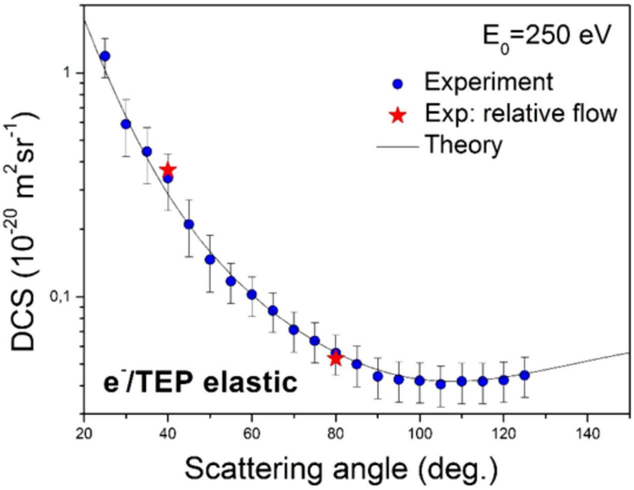

Fig. 3. The same as in Figure 2 but for 250 eV incident electron energy. The reference points for Ar are taken from paper Williams and Willis [11].

Table 1. Experimentally obtained DCSs for elastic electron scattering form TEP as a function of scattering angle at fixed electron energies. Total absolute errors rounded to the last two significant digits are given in brackets.

θ (°)	DCS (10^{-20} m^2sr^{-1})				
	50 (eV)	100 (eV)	150 (eV)	200 (eV)	250 (eV)
25	–	2.08(43)	1.90(39)	1.61(46)	1.19(24)
30	4.4(1.2)	1.09(31)	0.95(27)	0.78(21)	0.59(17)
35	2.57(74)	0.79(23)	0.57(16)	0.54(15)	0.44(13)
40	2.05(42)	0.53(15)	0.41(12)	0.41(12)	0.993(96)
45	1.49(31)	0.466(97)	0.318(91)	0.312(89)	0.211(60)
50	1.12(23)	0.369(77)	0.255(73)	0.213(61)	0.147(42)
55	0.82(17)	0.302(63)	0.198(56)	0.159(46)	0.117(23)
60	0.62(13)	0.243(51)	0.151(43)	0.132(38)	0.102(21)
65	0.49(10)	0.201(42)	0.123(25)	0.120(25)	0.087(18)
70	0.409(84)	0.162(34)	0.106(22)	0.111(23)	0.071(14)
75	0.354(73)	0.313(27)	0.097(20)	0.099(21)	0.064(13)
80	0.312(64)	0.113(24)	0.093(19)	0.088(18)	0.056(11)
85	0.279(58)	0.107(22)	0.091(18)	0.081(17)	0.050(10)
90	0.259(54)	0.109(23)	0.085(17)	0.077(16)	0.0441(90)
95	0.256(53)	0.115(24)	0.083(17)	0.073(15)	0.0427(88)
100	0.260(54)	0.126(26)	0.083(17)	0.068(14)	0.0423(86)
105	0.285(59)	0.139(29)	0.088(18)	0.070(14)	0.0407(84)
110	0.326(67)	0.155(32)	0.092(19)	0.069(14)	0.0420(86)
115	0.382(79)	0.171(36)	0.095(19)	0.072(15)	0.0419(86)
120	0.471(97)	0.192(40)	0.103(21)	0.077(16)	0.0425(87)
125	0.59(12)	0.217(45)	0.109(22)	0.084(17)	0.0446(91)

5 Conclusion

Elastic scattering of electrons from triethyl phosphate molecule is investigated experimentally and theoretically in the energy range from 50 eV to 250 eV. The relative DCSs are measured as a function of scattering angle at fixed incident electron energies. The relative flow method is used for calibration of relative results on absolute scale, using argon as a referent gas. Experimental measurements are compared with the calculations, which are obtained using Independent Atom Model (IAM), and good agreement is noticed.

In an attempt to develop more efficient radiation-based technologies and for better comprehension of the radiation damage of biomolecules, a deeper understanding of fundamental processes at the molecular level is needed, which implies electron interactions with molecules that form the medium. For this reason, the results from this paper can be of interest since they contribute to a fundamental understanding of the electron interaction with a relatively large molecule.

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Author contribution statement

Q1 Please note that you are required to include a statement which details the nature of the contribution of each author.

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Elastic electron differential cross sections for argon atom in the intermediate energy range from 40 eV to 300 eV

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Regular Article

Elastic electron differential cross sections for argon atom in the intermediate energy range from 40 eV to 300 eV[⋆,⋆⋆]

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Abstract. Measurements and calculations for electron elastic differential cross sections (DCS) of argon atom in the energy range from 40 to 300 eV are presented. DCS have been measured in the crossed beam arrangement of the electron spectrometer with an energy resolution of 0.5 eV and angular resolution of 1.5° in the range of scattering angles from 20° to 126°. Both angular behaviour and energy dependence of DCS are obtained in a separate sets of experiments, while the absolute scale is achieved via relative flow method, using helium as a reference gas. All data is corrected for the energy transmission function, changes of primary electron beam current and target pressure, and effective path length (volume correction). DCSs are calculated in relativistic framework by expressing the Mott's cross sections in partial wave expansion. Our results are compared with other available data.

1 Introduction

Electron elastic differential cross sections (DCS) of argon atom have been investigated thoroughly in the past by many experimental groups and different theoretical approaches but they still need further analysis and improvements. There are numerous reasons for this study: (i) DCS is still one of the stringiest test for electron–atom interaction that is energy (E_o) and angle (θ) dependent and where different theoretical approximations work adequately only in a certain (E_o, θ) domain. DCS is one of the variables in the "perfect scattering experiment" which has to be determined in absolute values in order to reproduce all complex scattering amplitudes [1]; (ii) Argon atom is often used as a model for both experimental (easy to handle, inexpensive in high purity) and theoretical (closed shell, many electron system) studies. Recently, Bartschat et al. [2] used an argon atom to make an overview on quantum-mechanical approaches for generating the electron–atom cross sections and to perform uncertainty estimates; (iii) atomic argon is an important model for the numerous calculation codes, now available, which use either quantum chemistry codes [3] or through other codes, like relativistic Dirac partial-wave analysis, incorporated into databases [4]; an important model for all being argon atom; (iv) there is a need for accurate cross sections for argon atom in experiments that use relative flow method (RFM) to determine absolute values of DCS for more complex molecules [5]. One of the key requirements in RFM is to provide similar flowing conditions (special distributions) of the measured and reference gas. This is easier to achieve if the masses of gases are similar, hence Ar or N_2 gases are preferentially used as references rather than helium which has the best known literature values for DCSs; and (v) the authors want to extend previous DCS measurements on Ar (listed in Tab. 1 among the other e/Ar data).

The first measurements of the differential electron elastic scattering by argon atom include those performed in 1931 by Bullard and Massey [6] and by Arnot [7] where the angular distributions were obtained in the ranges 4–40 eV, 15°–125° and 42–780 eV, 20°–120°, respectively. A comprehensive review of later experimental and theoretical results on electron/Ar cross sections up to 1995 was given by Zecca et al. [8] and results up to 2002 were compiled by Raju [9]. A critical data evaluation and consistency of electron scattering by argon was made in 2008 by Gargioni and Grosswendt [10]. A comparison of sets of cross sections for electron scattering from ground-state Ar in the energy range from thermal to about 1 keV with the overview of cross sections maintained by LXCAT database is given in [11]. The most recent results are presented in Table 1. The present experiment covers the electron impact energy range from 40 eV to 300 eV and the scattering angles from 25° up to 126°, while calculations are performed in broader range of impact energies and for the full range of scattering angles.

[⋆] Contribution to the Topical Issue "Physics of Ionized Gases (SPIG 2016)", edited by Goran Poparic, Bratislav Obradovic, Dragana Maric and Aleksandar Milosavljevic.

[⋆⋆] Supplementary material in the form of one pdf file from the Journal web page at `https://doi.org/10.1140/epjd/e2017-80677-4`.

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Table 1. The latest experimental and theoretical work on DCS for elastic cross section for argon atom covering impact energy range from 40 to 300 eV.

Author	Type of experiment/ theoretical approach	Energy range (eV)	Angular range (°)
Paikeday and Alexander [12]	Model potential	20–500	0–180
Kelemen [13]	Optical potential	0.5–500	Spin polarisation 0–180
Blanco and García [14]	Quasifree nonempirical model	40–10 000	0–180
Blanco and García [15]	Quasifree nonempirical model	40–800	0–180
Salvat [16]	Optical-model potential	100–3000	0–180
Milosavljević et al. [17]	Crossed beams/ relativistic ab initio	40–150	40–126
Yousif Al-Mulla [18]	Local density approximations	10–100	0–180
Jablonski et al. [19]	Thomas–Fermi–Dirac/ Dirac–Hartree–Fock potential	50–3000	0–180
Adibzadeh and Theodosiou [20]	Relativistic/nonrelativistic phase shifts	5–1000	0–180
Hargreaves et al. [21]	Crossed beams (SSRDM)	20–50	20–135
McEachran and Stauffer [22]	Ab initio optical potential	40–100	0–180
Bote et al. [23]	Optical-model potential	10–3000	0–180

2 Experimental method and theoretical approach

2.1 Experimental set-up

The home-made experimental setup is based on a crossed-beam technique comprising of an electron gun, a single capillary gas needle and a detection system with single channel electron multiplayer detector (channeltron). Detailed description of the original setup is given in [24,25], while construction of a gas line used for relative flow technique, design and programming of digital acquisition system are detailed in [5]. Briefly, electrons are produced from an indirectly heated thoriated tungsten hairpin filament (diameter 0.2 mm). Emitted electrons are then doubly focused by a 9 electrode system of the electron gun, including two axis deflector electrodes. The energy resolution of electrons at the exit of the electron gun is limited by a thermal distribution of emitted electrons to about 0.5 eV as there is no monochromaticity. The electron gun is mounted on a turntable and can be rotated in the plane of scattering from −40° to 126° around the fixed detection system. The angular resolution is estimated to about ±1.5°, while the zero angle uncertainty is better than ±0.25° regarding the alignment and center precision of the entire system. The distance from the last electrode of the electron gun to the scattering centre (gas needle) is 30 mm, while the interaction volume is about 3 mm above the gas needle. The aspect ratio of the effusive beam capillary is 0.0125 with a length of 40 mm. The detection system consist of four electrode lens at the entrance of a double cylindrical mirror analyser (DCMA), three electrode lens at its exit and PHOTONIS X810BL channeltron enclosed in a shielded case. The first electrode of a four electrode lens is positioned 25 mm from the gas needle. Its function is to focus the scattered electrons and to apply the retarding potential such that electrons always have a fixed energy when entering DCMA. Therefore, DCMA is operated in a constant pass energy mode with an energy resolution down to about 0.4 eV.

2.2 Measurement procedure

DCS data as function of scattering angle, DCS (θ), is obtained by measuring the signal and background for each angle point. The signal measurement is performed first and is followed by background measurement, which involves the introduction of a target gas into the chamber from the side leak, whilst the signal is measured for target gas diverted through the gas needle. These two measurements were performed at least three times for each electron energy of interest. Subtracting the background from signal yields three corrected measurements which were weighted and averaged. For each electron energy, the analyser was set to allow the electrons corresponding to the elastic peak to pass through. Accordingly, the electron gun and two lenses before and after the analyser were readjusted for optimal signal and to compensate for the transmission functions.

DCS data as a function of electron energy, DCS (E_o), is obtained by fixing the angle and measuring the count for each energy point for at least three times. Prior to this measurement, the electron current in a Faraday cup as a function of electron energy was recorded, even though the electron gun was refocused. The transmission of the analyser system as a function of electron energy has been obtained from a simulation in SIMION8 [26], where optimal lens potentials were determined. These potentials were then used for the measurements and the obtained data was normalized to the simulated transmission. Additional normalization was performed to compensate for the small change in the gas needle pressure over time and measured electron current.

The relative flow measurements were taken for the needle pressure of about 0.373 mbar for Argon (target gas) and about 0.133 mbar for Helium (buffer gas). The ultimate base pressure in the experiment was about 5×10^{-7} mbar, while working pressure when both gasses were introduced in the chamber was in the order of 5×10^{-6} mbar. Each relative flow measurement was performed two times and the average values were taken for the normalization to absolute scale.

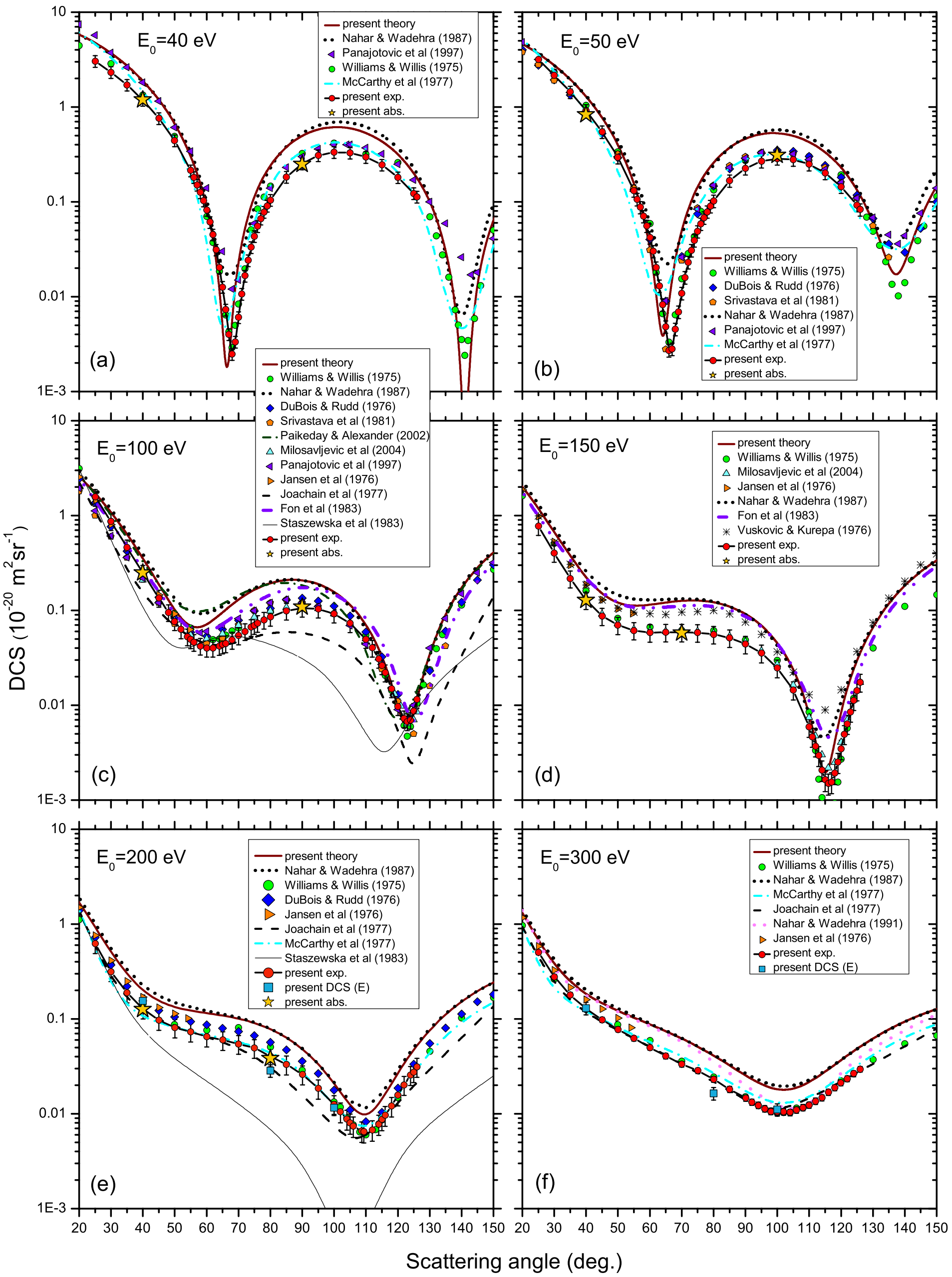

Fig. 1. Angular behaviour of differential cross section for elastic scattering of electrons on argon. The present experimental and theoretical data are compared with the selected set of previous results. The data symbols used correspond to: (red circles), present experiment; (yellow stars), present absolute data from relative flow; (dark cyan squares), present DCS (E); (dark red full line), present theory; (green circles), Williams and Willis [30]; (orange right triangles), Jansen et al. [31]; (asterisk); Vušković and Kurepa [32]; (blue diamond), DuBois and Rudd [33]; (dashed line), Joachain et al. [34]; (cyan dash dot line), McCarthy et al. [35]; (orange pentagons), Srivastava et al. [36]; (violet dash dot line), Fon et al. [37]; (thin line), Staszewska et al. [38]; (dotted line), Nahar and Wadehra [39]; (magenta short dash line), Nahar and Wadehra [42]; (violet left triangle), Panajotović et al. [44]; (olive dash dot line), Paikeday and Alexander [12]; (cyan up triangles), Milosavljević et al. [17].

2.3 Normalization and experimental uncertainties

The relative DCS data is made absolute by using the relative flow technique with Helium as a reference gas. Data for Helium was taken from Register et al. [27] and both DCS (θ) and DCS (E_o) were measured at least three times and the weighted average as well as weighted uncertainties were calculated. To this statistical uncertainty, the instrumental uncertainties (effective path length correction, uncertainty in energy and angular scale) and the uncertainty from a normalization originating from the relative flow measurements and Helium data, specified by the authors, was added. The total uncertainties vary with impact electron energy and span from 14% at the lowest up to 22% for the highest impact energy.

Table 2. Experimental and theoretical DCS for elastic cross section for argon atom used for a comparison with present results.

Author	Type of experiment/ theoretical approach	Energy range (eV)	Angular range (°)
Williams and Willis [30]	Modulated crossed beam	20–400	20–150
Jansen et al. [31]	Gas cell	100–3000	5–55
Vušković and Kurepa [32]	Gas cell	60–150	5–150
DuBois and Rudd [33]	Gas cell	20–800	2–150
Joachain et al. [34]	Optical potential	100–800	
McCarthy et al. [35]	Optical potential	20–3000	
Srivastava et al. [36]	Crossed beams (RFM/He)	3–100	20–135
Fon et al. [37]	*R*-matrix	3–150	
Staszewska et al. [38]	Quasifree-scattering model/ optical-model potential (SEPa)	30–3000	
Nahar and Wadehra [39]	Model potential	3–300	
Salvat et al. [40]	Semiphenomenological approach	100–5000	
Bartschat et al. [41]	Optical potential method	15–100	
Nahar and Wadehra [42]	Relativistic Dirac equation	3–300	
Cvejanović and Crowe [43]	Crossed beams	20.4–110	40–120
Panajotović et al. [44]	Crossed beams	10.3–100.3	20–150

RFM/gas – relative flow method with gas used as a reference; SEP – static, exchange, polarisation, absorption potential.

2.4 Calculations

The partial expansion method was used to describe the differential and total cross sections for elastic scattering. The relativistic differential cross section per unit solid angle is given by sum of squares of the direct $f(\theta)$ and spin-flip $g(\theta)$ scattering amplitudes:

$$\frac{d\sigma_e}{d\theta} = |f(\theta)|^2 + |g(\theta)|^2, \tag{1}$$

where θ denotes the scattering angle $f(\theta) = \sum_{l=0}^{\infty} F_l P_l(\cos(\theta))$, $g(\theta) = \sum_{l=0}^{\infty} G_l P_l^1(\cos(\theta))$, $P_l(\cos(\theta))$ are the Legendre polynomials, $P_l^1(\cos(\theta))$ are the associated Legendre functions. F_l and G_l can be calculated as follows:

$$F_l = \frac{1}{2ik}\left\{(l+1)\left[\exp\left(2i\delta_{l+}\right)-1\right] + l\left[\exp\left(-2i\delta_{l-}\right)-1\right]\right\}$$

$$G_l = \frac{1}{2ik}\left[\exp\left(2i\delta_{l-}\right) - \exp\left(-2i\delta_{l+}\right)\right],$$

where δ_{l+}, δ_{l-} are the phase shift of the order l, and k is the momentum of the projectile electron. Details of the calculations can be found in reference [29]. The total elastic cross section, σT, can be obtained after integration over the all possible scattering angles as:

$$\sigma_T = 2\pi \int_0^{\pi} \frac{d\sigma_e(E_o,\theta)}{d\Omega} \sin\theta \, d\theta. \tag{2}$$

3 Results and discussion

3.1 Angular behaviour of differential cross sections, DCS (θ)

Differential cross sections for electron elastic scattering by argon atom, DCS (θ), at impact energies of 40, 50, 100, 150, 200 and 300 eV are shown in Figure 1. The present experimental results are obtained from three separate sets of measurements: the direct angular distribution measurements over whole accessible angular range; data points at fixed angles derived from relative flow measurements with helium as a reference gas; and the direct measurements of energy dependence at fixed scattering angle. The first and third sets give the relative values, while the second set gives the absolute values. Relative sets are made absolute by fitting the curves to absolute data points by the least squares method. Present experimental and theoretical DCS are compared with other data listed in Table 2. Experimental values of DCS are tabulated in Table 3 with the quoted level of uncertainties.

The differential cross section at 40 eV exhibits two pronounced minima, at 68° and 142°. The excellent agreement between present measurements and former absolute measurements of Williams and Willis [30] is found. The value of the DCS at the first minimum is $(2.50 \pm 0.15) \times 10^{-23}\,\mathrm{m^2/sr}$ and is as low as reported in [30]. The position of the minimum also agrees with the measurements of Panajotović et al. [44], but their minimum is less pronounced. The difference could be due to the proximity of the critical point in argon (around 41.30 ± 0.02 eV; $68.5° \pm 0.3°$ [44]), although even at the critical point, their minimal value is only $(6.1 \pm 1.3) \times 10^{-23}\,\mathrm{m^2/sr}$. This can indicate the importance of subtraction of the residual background gas obtained by diverting gas through a side leak, as explained in Section 2.2.

The present calculations have the best agreement with the calculations of Bartschat et al. [41] in both absolute values and positions and depth of minima. Calculated DCS first minimum is almost of the same absolute value, just shifted to lower scattering angle of 66.4° compared to the present measurements. The calculated values at smaller scattering angles are higher than the experimental results but agree with previous measurements in [44]. The

Table 3. Experimental DCS for elastic cross section for argon in units of 10^{-20} m^2/sr with the relative uncertainties indicated for each impact energy.

Angle (°)	10^{-20} m^2 sr^{-1}					
	40 eV	50 eV	100 eV	150 eV	200 eV	300 eV
25	3.051	3.172	1.57	0.7762	0.6212	0.504
30	2.328	2.17	0.869	0.4039	0.316	0.277
35	1.711	1.442	0.461	0.2168	0.1888	0.1794
40	1.185	0.919	0.248	0.1289	0.1273	0.128
45	0.762	0.5475	0.135	0.0872	0.0972	0.098
48			0.0952			
50	0.444	0.2956	0.0765	0.07	0.081	0.0776
52			0.063			
54			0.053			
55	0.215	0.1314	0.0495	0.0615	0.073	0.0625
56	0.182	0.1067	0.0462			
57	0.151	0.0878				
58	0.126	0.0705	0.0422			
59	0.103	0.0558				
60	0.0820	0.0421	0.0401	0.0585	0.0649	0.0501
61	0.0612	0.0301				
62	0.0452	0.0202	0.0402			
63	0.0313	0.0130				
64	0.0204	0.0083	0.042			
65	0.0126	0.0048	0.0436	0.0588	0.0599	0.0406
66	0.0073	0.0027	0.0449			
67	0.004	0.0028				
68	0.0025	0.0046	0.0489			
69	0.0034	0.0069				
70	0.0061	0.0109	0.0543	0.0588	0.0545	0.0334
71	0.0107	0.0159				
72	0.0166	0.0231	0.0601			
73	0.0242	0.0309				
74	0.0332	0.0393	0.0666			
75	0.0435	0.0488	0.0699	0.0583	0.0495	0.0285
76	0.0554	0.0586	0.0733			
77	0.0663	0.0682				
78	0.0782	0.0788	0.0792			
79	0.0908	0.0902				
80	0.105	0.1024	0.0855	0.0559	0.0404	0.0231
85	0.183	0.1672	0.0989	0.0515	0.0332	0.0181
90	0.253	0.2265	0.1059	0.0442	0.026	0.0146
92						0.0133
94						0.0123
95	0.309	0.2674	0.1036	0.0355	0.0186	
96						0.0113
98						0.0106
100	0.334	0.2863	0.092	0.0247	0.0126	0.0105
102					0.0105	0.0105
104					0.0088	0.0103
105	0.3295	0.2792	0.073	0.0145	0.008	
106					0.0074	0.011
108					0.0066	0.0116
110	0.297	0.249	0.0497	0.0059	0.0065	0.0124
111				0.0047		
112			0.0403	0.0037	0.0068	0.0136
113				0.003		
114			0.0308	0.0021	0.0078	0.0147
115	0.246	0.2018	0.0263	0.0016	0.0087	
116			0.0221	0.0015	0.0097	0.0168
117				0.0016		
118			0.015	0.0019	0.0121	0.0189
119				0.0025		

(continued...)

Table 3. *(continued...)*

Angle (°)	10^{-20} m^2 sr^{-1}					
	40 eV	50 eV	100 eV	150 eV	200 eV	300 eV
120	0.181	0.1446	0.0097	0.0035	0.0157	0.0212
121				0.005		
122			0.0073	0.0064	0.0202	0.0234
123			0.0067	0.0085		
124			0.007	0.0113	0.0257	0.0265
125	0.123	0.0927	0.0087	0.0142	0.0275	
126	0.113	0.083	0.0115	0.0175	0.0313	0.0295
Relative uncertainty (%)	14	15	20	20	21	22

local maximum around 100° is larger than other experimental values and calculations of McCarthy et al. [35] but it is close to the values of Nahar and Wadehra [39]. The second minimum is found at 141° and is much deeper than both calculated [35] and measured [30,44] values.

The present experimental DCS at 50 eV agrees perfectly with previous measurements [30,33,36,44] in the whole angular range. The position and the value of the first minimum at 67° is the same as in [30,36]. The second minimum is beyond the angular range of the present experiment. The calculated DCS at 50 eV matches the experimental values at smaller scattering angles but has the minimum at 64.1°. Again at local maximum, the DCS is larger and has the same value as in [39]. The positions of both minima are close to other calculations [35,39] but with smaller values.

There are many experiments and theories for 100 eV impact energy. All experiments have an excellent agreement, at local maximum of 90° with discrepancy within ±15%. The present calculated values agree with other calculations [12,37,39] except when compared to calculations by Joachain et al. [34] whose values are smaller in the whole angular range. The values of the calculations of [34] agree very well with the present measurements at the position of the first minimum. The present calculated values in the range of the second minimum strongly agree with the previously measured values in our laboratory by Milosavljević et al. [24].

There are two sets of previously measured data for 150 eV: Jansen et al. [31]; Vušković and Kurepa [32]; and Milosavljević et al. [24]; Williams and Willis [30]. The main distinction is in the values of the plateau at around 70° where the DCS has a flexing point (the first minimum became very shallow at this energy) and the DCS values of the first group are larger for 60% than the vales of the second group. Interestingly, the present calculated values and those in [39] are even larger (factor 2.14) and they better match the experiments of the first group [31,32] while the present experiment favors the second group of results [24,30]. At this impact energy the second minimum is within the accessible range of the present experiment and its position at 116° agrees well with [24,30] – the present calculation gives the position of 115.1°. Also, the values of present measurement and calculation agree very well – in contrast with previous calculations [37,39] where the shallower minimum was obtained.

At 200 eV, the shapes and the values of all experiments and calculations, except for calculations by Staszewska et al. [38] and Salvat et al. [40], are virtually the same and all DCSs lay within ±40% band around mean value. For both impact energies of 200 eV and 300 eV, the present calculations agree excellently with calculations of [39] in the full angular range, but they exceed the experimental values. Inclusion of imaginary part in the Dirac potential brought the calculations at 300 eV in [42] in agreement with experimental values in the region of the minimum when compared to the previous nonrelativistic calculations of the same authors [39]. Still, these relativistic calculations are much higher than experiments at middle angles (50°–80°) where they agree with the present calculations based on the Mott's cross sections.

3.2 Energy dependence of differential cross sections, DCS (E_o)

Differential cross sections dependence on the impact energy, DCS (E_o), at fixed scattering angles of 40°, 80° and 100° are presented in Figures 2a–2c, respectively. Two sets of present experimental points are shown: the direct energy scans corrected for the analyser transmission and primary beam current and the single data points of relative flow measurements where absolute scale was established by helium data comparison [27]. Present experimental data are compared with other direct energy scan measurements of Cvejanović and Crowe [43]. The excellent agreement is found for all three scattering angles at the overlapping energies (40–100 eV). It is worth noting that the absolute scale of these two measurements have been established in different way, in [43] data have been normalized to previous absolute data of Srivastava et al. [36] while the present data were normalized on reference helium gas data obtained in a separate set of present measurements.

Present calculations generally give larger cross sections than experimental measurements, particularly at 100° and energies above 100 eV. This could be due to the sensitivity of DCS (E_o) at this angle because of the proximity of the

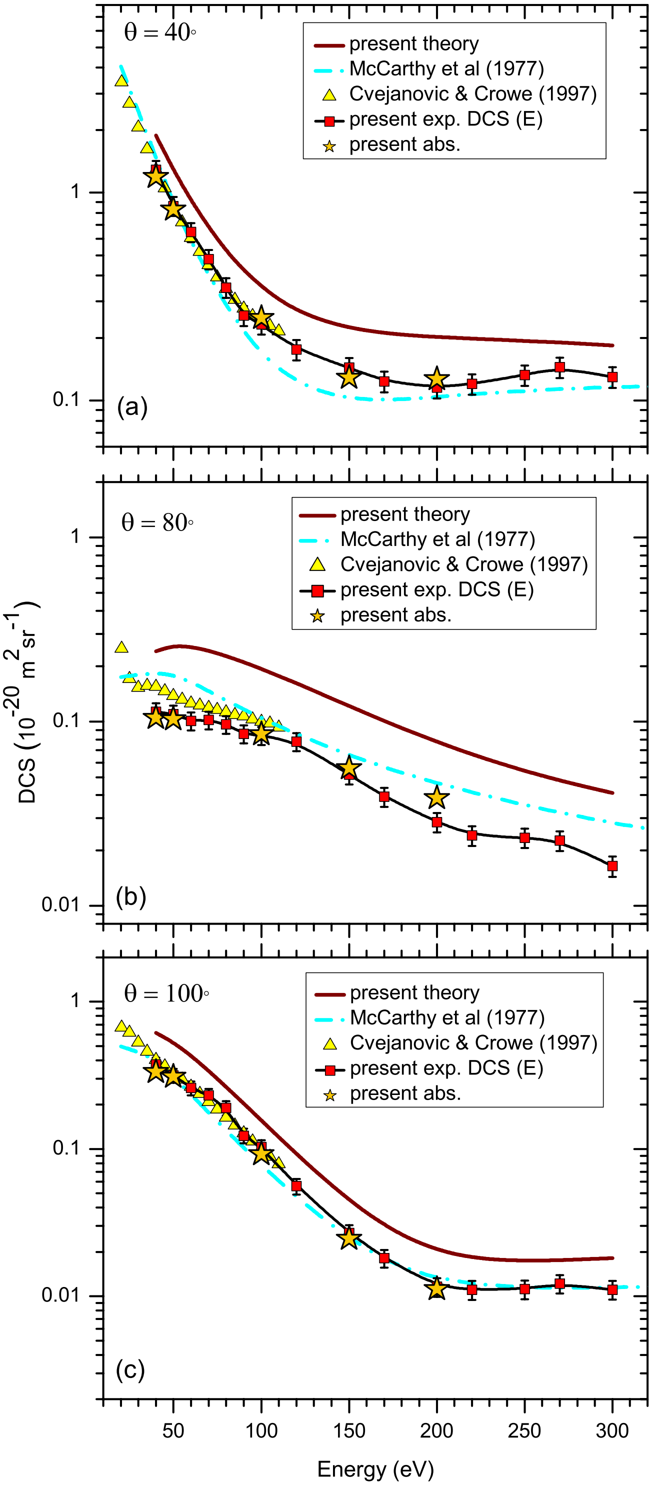

Fig. 2. Comparison of the present energy dependence of the differential cross section for elastic scattering of electrons on argon at a scattering angles of: (a) 40°; (b) 80° and (c) 100° with previous experimental and theoretical results. Error bars corresponding to the quoted uncertainties are presented on present data points. The data symbols used correspond to: (red squares), present experiment DCS (E); (yellow stars), present absolute data from relative flow; (dark red full line), present theory; (cyan dash dot line), McCarthy et al. [35]; (yellow up triangles), Cvejanović and Crowe [43].

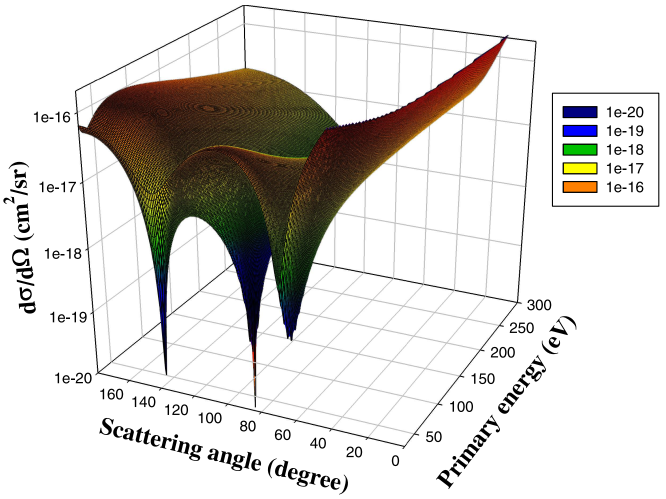

Fig. 3. Calculated differential cross section surface for electron elastic scattering by argon in the energy range from 40 to 300 eV. The full data set is given in the Supplementary material.

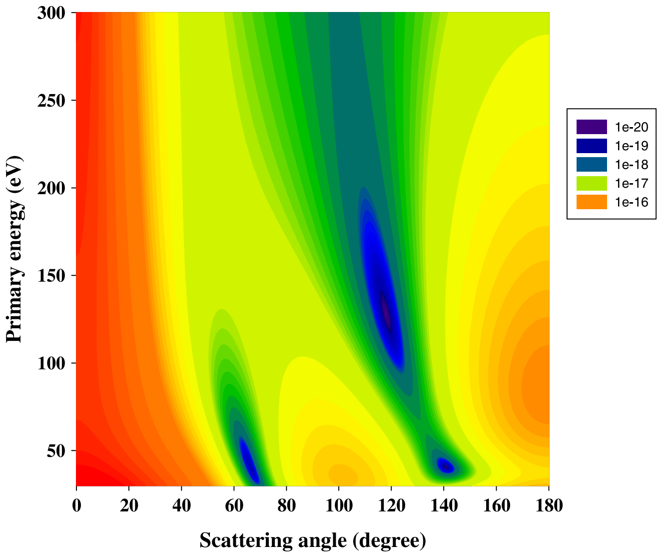

Fig. 4. Projection of 3D surface of elastic DCS for argon on the plane scattering angle – primary electron energy.

minimum point. The calculations of McCarthy et al. [35] agree better with the present measurements.

3.3 Differential cross section surface, DCS (E_o,θ), minima positions and critical points

It has been previously pointed out by Milosavljević et al. [25] that is of great importance to perform measurements of differential cross sections as independent energy and angular scans. This results in the whole DCS (E_o,θ) surface being crossed-checked so that experimental errors could be avoided. These errors include energy transmissions of electron gun and analyser as well as misalignment

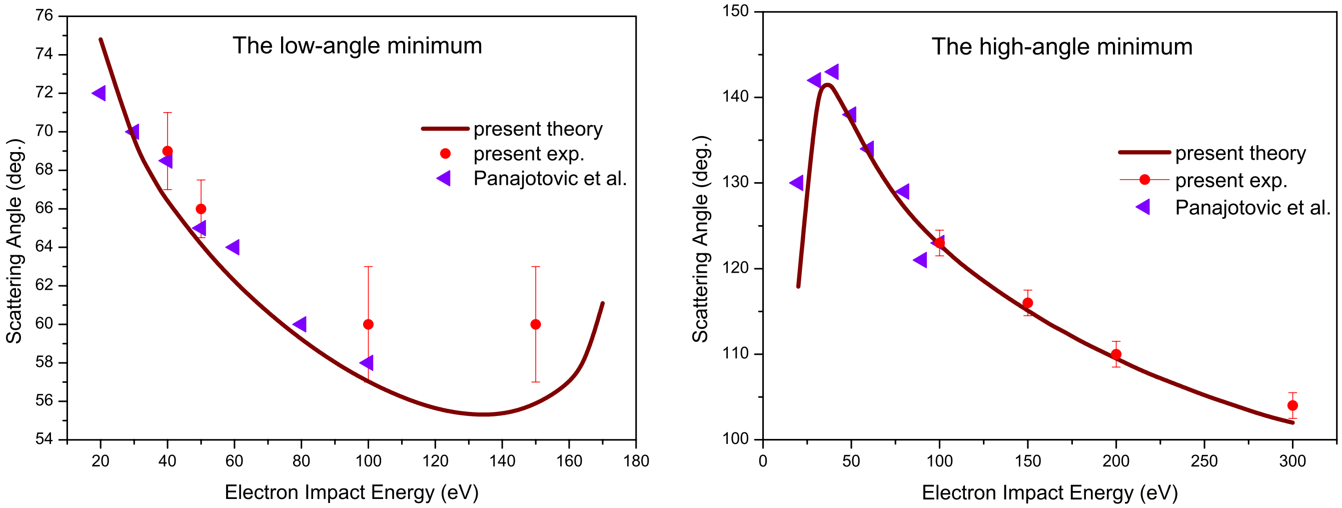

Fig. 5. Positions of low-angle and high-angle minima versus electron impact energy. The data symbols used correspond to: (red circles), present experiment; (dark red full line), present theory; (violet left triangle), Panajotović et al. [44].

of three axis, the primary beam axis, the target beam axis and the analyser axis.

In order to obtain the full 3D plot of the differential cross section surface it is necessary to calculate or measure differential cross sections on a rather dense grid, hence the present calculations being performed in angular steps of 0.1° and energy steps of 0.1 eV. The obtained surface is presented in Figure 3.

In the energy range from 30 to 300 eV differential cross sections show three critical points – places in 3D surface where DCS reach a minimum. The determination of these points is important as the critical minima represent a sensitive test of the interplay between direct and exchange potentials in electron interaction with the target atom. In the vicinity of critical minima the scattered electrons exhibit the largest change of the polarisation. Finding the pairs of incident energy and scattering angle where DCS minima attain their smallest values is a tedious task in experimental study and in the same time represents a crucial test of applied approximations in calculations. A detailed analysis of critical points in argon has been done by Lukas [45] and more recently by Sienkiewicz et al. [46] using ab initio relativistic calculations. Experimental values found in [44] are (37.30 ± 0.02 eV, 143.5° ± 0.3°) and at (41.30 ± 0.02 eV, 68.5° ± 0.3°) and the third minimum in [24] to be at (129.4 ± 0.5 eV, 119.4° ± 0.5°). The present calculations also reveal the positions of three critical points clearly shown in Figure 4. Positions of critical minima in the present calculations are found to be: (41 eV, 141°), (41 eV, 66°) and (128 eV, 118°). It could be compared with the previous calculations in [46] (39.3 eV, 68.0°), (39.5 eV, 141.0°) and with calculations presented in [24] (118.0 eV, 118.9°).

The positions of low-angle and high-angle minima could also be traced with the change of impact electron energy. The calculated values for the first and the second minimum with experimental points at fixed energies are shown in Figures 5a and 5b, respectively.

4 Conclusions

Absolute measured and calculated differential cross sections for electron elastic scattering by argon atom are presented. Measurements have been taken in the energy range from 40 eV to 300 eV and for scattering angles from 25° to 126°, with smaller steps around minima positions. Calculations were performed using relativistic expression of a partial wave expansion method for electron–atom scattering using the Mott's cross sections. Calculations have been performed in the energy range from 30 eV and for the full range of scattering angles, with the dense grid around critical points and positions of minima. The achieved agreement with other experiments and calculations is moderate and depends on impact energy and angular range. This indicates that advances in both experimental methods and applied theoretical approximations are required, despite the topic having been studied for a long time. It should not be forgotten that the differential cross sections and their absolute values are the crucial quantities in our quantum mechanical description of electron–atom interactions. We have achieved one of the goals, i.e. to provide a consistent set of data in this energy range that can be used in further experiments with other more complex targets, like biomolecules. All presented data, will be also maintained in the Belgrade electron/atom (molecule) database (BEAMDB) (http://servo.aob.rs/emol) [47].

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Author contribution statement

MLjR and JBM performed the experimental measurements, TK made all calculations, BPM, MLjR and TK wrote the manuscript. All authors discussed the results and commented on the manuscript.

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Elastic Electron Scattering from Methane Molecule in the Energy Range from 50–300 eV

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Abstract: Electron interaction with methane molecule and accurate determination of its elastic cross-section is a demanding task for both experimental and theoretical standpoints and relevant for our better understanding of the processes in Earth's and Solar outer planet atmospheres, the greenhouse effect or in plasma physics applications like vapor deposition, complex plasma-wall interactions and edge plasma regions of Tokamak. Methane can serve as a test molecule for advancing novel electron-molecule collision theories. We present a combined experimental and theoretical study of the elastic electron differential cross-section from methane molecule, as well as integral and momentum transfer cross-sections in the intermediate energy range (50–300 eV). The experimental setup, based on a crossed beam technique, comprising of an electron gun, a single capillary gas needle and detection system with a channeltron is used in the measurements. The absolute values for cross-sections are obtained by relative-flow method, using argon as a reference. Theoretical results are acquired using two approximations: simple sum of individual atomic cross-sections and the other with molecular effect taken into the account.

Keywords: methane; cross-section; elastic scattering; electrons

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1. Introduction

Methane (CH_4) is the simplest alkane. Its molecule has tetrahedron shape, belongs to the T_d point group symmetry, and does not possess dipole and quadrupole moments. Furthermore, methane is widely distributed in the Solar System. In general, the inner planets Mercury [1], Venus [2], and Mars [3] are methane-poor, except Earth, whereas outer planets Jupiter [4], Saturn [5], Uranus [6], and Neptune [7] have methane-rich atmospheres. Currently, the methane levels in Earth's atmosphere are around 1.6–1.8 ppmv and are considered one of the main causes of the greenhouse effect. Greenhouse effect caused by methane is about eight times that of CO_2 [8]. Emission of CH_4 in atmosphere is about 40% from natural, and about 60% from anthropogenic sources (agriculture, energy, and waste sectors [9]). In past decades methane's growth rate was changing, and in recent years, it has been increasing [10]. That is a reason why investigation of this gas again becomes consequential.

Electron collisions with methane are very important in plasma physics. In mixture with hydrogen and argon, CH_4 is used for r. f. plasma-enhanced chemical vapor deposition (R. F. PECVD) of nanocrystalline diamond films [11]. On the other hand, methane is less used than silane in design of solar cells. Its use in the preparation of amorphous SiC *p*-layers is most often emphasized in a PECVD process using high R.F. power at relatively low temperature [12]. When a Tokamak is operated at high density and high temperature methane plays a dominant role in the edge plasma region [13]. Particles and energy are expelled from the plasma and are transported to the vessel wall, which leads to complex

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plasma-wall interactions. These interactions create impurities in the plasma, including methane and its derivates, resulting in significant cooling of plasma, which can prevent achievement of rector relevant conditions. Therefore, understanding transport features of methane in plasma and interpretation of electron methane collisions in different physical processes plays a significant role in laboratory research in different fields of physics as well as in the investigation of properties atmospheres planets in Solar System. Finally, from a theoretical perspective and, because of its simplicity, methane can serve as a test molecule for advancing novel electron-molecule collision theories (e.g., Blanco et al. [14], Allan [15]).

Elastic electron scattering from methane molecule has been studied intensely in the past, and the most recent review of elastic differential cross-sections is given in [16]. Recommended set of data for electron/methane interactions is given by Song et al. [17]. For low incident electron energies (below 50 eV), elastic electron scattering from methane molecule has been studied experimentally and theoretically equally extensively. To cite few most recent papers, Allan [15] measured absolute differential elastic (impact electron energies 0.4–20 eV) and vibrational excitation cross-sections using an electron spectrometer with a magnetic angle changer, which allows measurements of differential cross-sections (DCSs) for backward angles. Bettega et al. [18] calculated DCSs and integral cross-sections (ICSs) for energies between 3 and 10 eV, using Schwinger multichannel method with pseudopotentials. Bundschu et al. [19] presented both experimental and theoretical results; measurements of DCSs using crossed beam apparatus and relative flow method, with He as a reference gas, and calculations using a body-fixed, single-center for close-coupled equations. Shyn and Cravens [20] reported DCSs for methane in energy range from 5 to 50 eV, using modulated crossed-beam method and He as reference gas for normalizing relative data to the absolute scale. At even lower electron energies, from 0.1 to 1.8 eV, an important study was one by Sohn et al. [21] where the references from even earlier measurements and calculations can be found. Several authors used R-matrix method to calculate cross-sections form methane [22–24].

As for papers that contain data for DCSs at intermediate-to-high energies ($E_0 \geq 50$ eV); Boesten and Tanaka [25] reported measured DCSs (electron energies between 1.5 and 100 eV), ICSs, and momentum transfer cross-sections (MTCSs) for methane. Measurements were done using crossed electron and molecular beam technique where observed DCSs were normalized point by point with the help of simultaneous measurements of DCSs of He. Vušković and Trajmar [26] obtained relative cross-sections for 20, 30, and 200 eV impact energies and normalized them to the absolute measurements of Tanaka et al. [27] for 20 and 30 eV, and to the calculations of Dhal et al. [28] for 200 eV. Cho et al. [29] published measured data for DCSs (ICSs and MTCSs as well) for electron elastic scattering from methane over scattering angles between 10° and 180° for incident electron energies from 5 to 100 eV using crossed beam spectrometer combined with a magnetic angle-changing device. Relative flow with He was exploited for normalization. They used the iterative Schwinger variational method combined with distorted-wave approximation to solve scattering equations. Sakae et al. [30] measured DCSs using crossed-beam method in angular range 5–135° for electron energies 75–700 eV. Relative DCSs were converted to the absolute values at 30° by using the ratio of elastic DCSs of the target gas to that of He. Iga et al. [31] used crossed beam apparatus to obtain scattering intensities (100–500 eV incident electron energies), which were converted to the absolute scale using relative flow method (Ne was used as a reference gas). Also, they used Schwinger variational method combined with the distorted-wave approximation to study elastic electron scattering (1–500 eV) theoretically. Jain [32] used a spherical optical complex potential model to investigate electron interaction with methane over a wide energy range from 0.1 to 500 eV. Mahato et al. [33] obtained analytical expressions for the static potentials of electron scattering from methane using Gaussian wave functions and studied elastic scattering from 10 to 500 eV incident electron energies utilizing those static potentials along with exchange and polarization potentials. Song et al. [17] presented recommended elastic DCSs and ICSs obtained by averaging other authors' data [15,19–21,25,29–31]. List of experimental and theoretical work on DCS for elastic electron scattering from methane molecule, in energy range of our interest is shown in Table 1. For the present work, the paper by Fuss et al. [34] is interesting because they provided the recommended set of data for differential and integral cross-sections for methane, including elastic electron scattering. They obtained their dataset by merging and averaging other authors' data [19,25,30,33] for lower energies and calculating ones for high energies (40–10 keV).

Table 1. List of experimental and theoretical work on differential cross-section (DCS) for elastic scattering of electrons from methane molecule, covering energy range from 50 to 300 eV.

Authors	Experiment Type with Normalization Method/Theoretical Approach	Energy Range (eV)	Angular Range (°)
Boesten and Tanaka [25]	Crossed beams, simultaneous measurements of DCS of He	1.5–100	10–130
Vušković and Trajmar [26]	Crossed beams, normalized to other authors results	20–200	8–130
Cho et al. [29]	Crossed beams, relative flow (He)/Schwinger variational method	5–100	10–180
Sakae et al. [30]	Crossed beams, relative flow (He)	75–700	5–135
Iga et al. [31]	Crossed beams, relative flow (Ne)/Schwinger variational method	100–500/ 1–500	10–135
Jain [32]	Spherical optical complex potential model	0.1–500	0–180
Mahato et al. [33]	Gaussian wave functions	10–500	0–180
Fuss et al. [34]	Optical potential method and the independent atom approximation including the screen corrected additivity rule (SCAR)	0.7–10,000	0–180

In this paper, theoretical and experimental results for elastic electron scattering from methane are shown. Obtained data include absolute differential cross-sections (DCSs) for elastic scattering for the incident electron energy range from 50 to 300 eV (with 50 eV steps) and angular range from 5° to 125° (with 5° steps), integral cross-sections, and momentum transfer cross-sections (ICSs and MTCSs, respectively) for every measured energy. The experiment was performed on a crossed-beam apparatus. As in most previous experiments [19,20,29–31], relative intensities were put on the absolute scale with help of relative flow method. The difference was in reference gas; in almost all experiments, He was used (except for Iga et al. [30] who used Ne), in our argon was reference gas. Theoretical results were obtained by calculating atomic cross-sections for molecular components, with two approximations used for molecular cross-sections simulations; simple sum (model 1) of atomic cross-sections and with molecular effect taken into the account (model 2). The existing variety of cross-section datasets for methane reflects our motivation to perform this study and, at the same time, to provide data at some of the impact energies where there are no previously measured data or where data require an independent confirmation. By exploiting different reference gas, Ar in this case, and performing new calculations that are using a coherent sum of atomic wave functions, we provide the independent and excessive datasets of cross-sections for this important molecule.

The paper is organized as follows. Theory and calculations of DCSs are explained in Section 2. Experimental setup and measurement procedure are given in Section 3. The obtained results are listed in Table 2 and presented graphically, including the comparison with the existing experimental and theoretical data, all given in Section 4. A discussion is given in Section 5. Finally, Section 6 is reserved for the conclusion.

Table 2. Experimental DCSs, integral cross-sections (ICSs), and momentum transfer cross-sections (MTCSs) for elastic scattering of electrons from methane molecule with absolute uncertainties Δ given in parentheses with 2 last digits. Values from 25° to 125° are measured and uncertainties arise from both statistical and short-term stability and include absolute uncertainties of cross-sections for reference Ar gas. Values from 0° to 20° and from 125° to 180° are extrapolated values and used to calculate ICSs and MTCSs. Uncertainties at small scattering angles are estimated to be 30%.

θ (°)	DCS (10^{-20} m^{2}sr^{-1})					
	50 (eV)	**100 (eV)**	**150 (eV)**	**200 (eV)**	**250 (eV)**	**300 (eV)**
0	17.5(5.3)	19.3(5.9)	25.1(7.9)	24.0(7.4)	24.5(7.0)	23.4(6.6)
5	13.8(4.1)	13.2(4.0)	15.8(4.7)	13.5(4.1)	12.9(3.9)	11.0(3.3)
10	9.8(2.9)	7.9(2.5)	7.9(2.5)	6.1(1.9)	5.0(1.4)	3.9(1.1)
15	6.3(1.9)	3.9(1.2)	3.2(1.0)	2.43(0.76)	1.50(43)	1.07(30)
20	3.7(1.1)	1.70(53)	1.09(35)	0.83(0.26)	0.43(12)	0.435(78)
25	1.96(60)	0.98(30)	0.45(14)	0.39(12)	0.325(93)	0.277(78)
30	1.30(40)	0.61(19)	0.277(87)	0.246(76)	0.200(57)	0.181(51)
35	0.73(22)	0.40(12)	0.194(61)	0.175(54)	0.136(39)	0.128(36)
40	0.50(12)	0.288(89)	0.162(51)	0.132(41)	0.106(22)	0.100(20)
45	0.384(88)	0.230(55)	0.127(31)	0.105(25)	0.072(15)	0.058(12)
50	0.302(70)	0.174(41)	0.090(22)	0.072(17)	0.053(11)	0.0423(85)
55	0.249(57)	0.128(30)	0.061(15)	0.055(13)	0.0413(85)	0.0347(70)
60	0.206(47)	0.091(22)	0.047(12)	0.044(10)	0.0324(67)	0.0264(53)
65	0.173(40)	0.068(16)	0.0398(99)	0.0362(88)	0.0271(57)	0.0214(43)
70	0.144(33)	0.055(13)	0.0340(84)	0.0306(74)	0.0229(48)	0.0186(38)
75	0.111(26)	0.0451(11)	0.0305(76)	0.0291(71)	0.0211(44)	0.0154(31)
80	0.092(21)	0.0409(98)	0.0283(70)	0.0252(61)	0.0181(38)	0.0120(25)
85	0.072(17)	0.0381(93)	0.0284(71)	0.0244(59)	0.0145(31)	0.0107(22)
90	0.067(16)	0.0403(96)	0.0263(66)	0.0212(52)	0.0121(26)	0.0096(20)
95	0.062(14)	0.043(10)	0.0274(68)	0.0195(48)	0.0120(26)	0.0088(18)
100	0.061(14)	0.047(11)	0.0256(64)	0.0183(45)	0.0118(26)	0.0088(18)
105	0.066(15)	0.049(12)	0.0252(63)	0.0185(45)	0.0106(23)	0.0085(18)
110	0.078(18)	0.051(12)	0.0250(62)	0.0160(39)	0.0099(22)	0.0078(16)
115	0.087(20)	0.057(14)	0.0250(62)	0.0154(38)	0.0094(21)	0.0078(16)
120	0.102(24)	0.061(15)	0.0260(65)	0.0155(38)	0.0092(20)	0.0073(15)
125	0.118(27)	0.063(15)	0.0264(66)	0.0141(35)	0.0092(20)	0.0075(16)
130	0.136(31)	0.066(16)	0.0258(63)	0.0139(35)	0.0092(20)	0.0072(15)
140	0.176(41)	0.071(17)	0.0249(61)	0.0140(35)	0.0091(20)	0.0066(14)
150	0.230(53)	0.074(18)	0.0244(61)	0.0142(35)	0.0089(20)	0.0061(13)
160	0.311(72)	0.077(18)	0.0243(61)	0.0144(36)	0.0086(19)	0.0059(12)
170	0.44(10)	0.079(19)	0.0243(61)	0.0144(36)	0.0084(19)	0.0058(12)
180	0.67(15)	0.079(19)	0.0243(61)	0.0145(36)	0.0083(19)	0.0057(12)
ICS's	6.1(1.8)	3.8(1.2)	2.95(0.92)	2.37(0.74)	1.89(0.55)	1.56(0.47)
MTCS's	2.09(0.53)	0.98(0.26)	0.45(0.13)	0.33(0.10)	0.222(0.054)	0.177(0.043)

2. Theory

In this work, the key to the determination of the elastic cross-section calculations of CH_4 is the atomic cross-section calculations for the components of the molecule. We assume for the determination of the effective interaction at distance **r** between a projectile electron and the target that the scattering potential can be expressed as:

$$V(r) = V_{\mathrm{st}}(r) + V_{\mathrm{ex}}(r) + V_{\mathrm{cp}}(r), \tag{1}$$

where V_{st} is the electrostatic potential, V_{ex} is the electron exchange potential and V_{cp} is the correlation-polarization potential. The electrostatic potential for the interaction between an electron and the target atoms:

$$V_{\mathrm{st}}(r) = -e[\varphi_{\mathrm{n}}(r) + \varphi_{\mathrm{e}}(r)], \tag{2}$$

where φ_n and φ_e are respectively the components of nucleus and the electron cloud of electrostatic potential.

The Furness-McCarthy exchange potential [35] is used for the electron exchange potential:

$$V_{\mathrm{ex,FM}}(r) = \frac{1}{2}[E - V_{\mathrm{st}}(r)] - \frac{1}{2}\left\{[E - V_{\mathrm{st}}(r)]^2 + 4\pi a_0 e^4 \rho_e(r)\right\}^{1/2}. \tag{3}$$

An accurate correlation-polarization potential combines the long-range polarization potential, $V_{\mathrm{cp,B}}(r)$, with the correlation potential $V_{\mathrm{cp}}(r)$ obtained from the local-density approximation (LDA) and it can be expressed as [36]:

$$V_{\mathrm{cp,LDA}}(r) \equiv \begin{cases} \max\{V_{\mathrm{cp}}(r), V_{\mathrm{cp,B}}(r)\}, & r < r_{\mathrm{cp}}; \\ V_{\mathrm{cp,B}}(r), & r \geq r_{\mathrm{cp}}. \end{cases} . \tag{4}$$

where r_{cp} is the outer radius at which $V_{\mathrm{cp}}(r)$ and $V_{\mathrm{cp,B}}(r)$ cross. The $V_{\mathrm{cp,B}}(r)$ when the projectile is far from the atom can be approximated by the Buckingham potential as:

$$V_{\mathrm{cp,B}}(r) = -\frac{\alpha_d e^2}{2(r^2 + d^2)^2}, \tag{5}$$

where α_d is dipole polarizability of the target atom and d is a phenomenological cut-off parameter that serves to prevent the polarization potential from diverging at $r = 0$. The experimental values of the atomic dipole polarizabilities from [37] are usually used in Equation (5). Perdew and Zunger [38] proposed a parameterization of the V_{cp}(r) correlation potential in the following form:

$$V_{\mathrm{cp}}(r) = \begin{cases} -\frac{e^2}{a_0}(0.0311 \ln r_s - 0.0584 + 0.00133 r_s \ln r_s - 0.0084 r_s), & r_s < 1; \\ -\frac{e^2}{a_0}\frac{0.1423 + 0.1748 r_s^{1/2} + 0.0633 r_s}{\left(1 + 1.0529 r_s^{1/2} + 0.3334 r_s\right)^2}, & r_s \geq 1. \end{cases} \tag{6}$$

where

$$r_s = \frac{1}{a_0}\left[\frac{3}{4\pi\rho_e(r)}\right]^{1/3} \tag{7}$$

is the radius of the sphere that contains (on average) one electron of the gas, in units of the Bohr radius a_0.

For the theoretical determination of the elastic cross-sections we used the Mott's differential cross-section [39],

$$\frac{d\sigma_e}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2, \tag{8}$$

where θ is scattering angle, $f(\theta)$ and $g(\theta)$ are the spin-up and spin-down scattering amplitudes. The $f(\theta)$ and $g(\theta)$ can be expressed as:

$$f(\theta) = \sum_{l=0}^{\infty} F_\ell P_\ell(\cos\theta), \tag{9}$$

$$g(\theta) = \sum_{l=0}^{\infty} G_\ell P_\ell^1(\cos\theta), \tag{10}$$

where $P_\ell(\cos\theta)$ are the Legendre polynomials, $P_\ell{}^1(\cos\theta)$ are the associated Legendre functions. The F_ℓ and G_ℓ can be calculated according to following relations:

$$F_\ell = \frac{1}{2ik}\left\{(\ell + 1)\left(e^{2i\delta_\ell^+} - 1\right) + \ell\left(e^{2i\delta_\ell^-} - 1\right)\right\}; \tag{11}$$

$$G_\ell = \frac{1}{2ik}\sum_{\ell=1}^{\infty}\left\{e^{2i\delta_\ell^-} - e^{2i\delta_\ell^+}\right\}, \tag{12}$$

where $\delta_\ell{}^+$ and $\delta_\ell{}^-$ are spin up and spin down phase shifts of the ℓth partial wave, and k is the momentum of the projectile electron, respectively.

The integration of the differential cross-section over total solid angles gives us the total elastic cross-sections in the following form:

$$\sigma_e = \int \frac{d\sigma_e}{d\Omega} d\Omega = 2\pi \int_0^\pi \sin\theta \left\{ |f(\theta)|^2 + |g(\theta)|^2 \right\} d\theta. \tag{13}$$

All calculations of elastic cross-section were performed by ELSEPA [40]. We used two approximations during the simulation of the molecular elastic cross-sections. In model 1, the calculated atomic cross-sections were simply added according to the stoichiometry numbers (additivity approximation). This approximation is frequently used approximation. However, it neglects the chemical-binding and aggregation effects. The electron distribution in molecules differs from that of an isolated atom of the same element. It was shown that this difference seems to have only a weak influence on the elastic DCS [40] at projectile energies larger than a few hundred eV. The effect of aggregation, the effect when the atoms are close together, has a stronger influence on the DCS [40]. In model 2 we have taken into account the positions of the atoms in the molecule. We used a single-scattering independent-atom approximation assuming that the interaction of the projectile with each atom of a molecule is given by the free-atom potential as for model 1. To determine the molecular DCS, the scattered wave at large distances from the molecule is approximated as the coherent sum of the wave functions scattered from all atoms in the molecule. In our calculations the carbon atom is located at the origin of the coordinate system. The positions of the hydrogen atoms are located at the following coordinates expressed in units of 10^{-10} m: $H_1(0.5541, 0.7996, 0.4965)$, $H_2(0.6833, -0.8134, -0.2536)$, $H_3(-0.7782, -0.3735, 0.6692)$, $H_4(-0.4593, 0.3874, -0.9121)$. We found the significant improvement in the cross-section calculations for model 2 compared with model 1.

3. Experiment

Experimental results presented in this paper are obtained on apparatus with crossed beams setting; incident electrons collide with a molecular beam perpendicularly. The experimental setup is placed inside the vacuum chamber, pumped with a turbomolecular pump to a typical background pressure (no gas in the chamber) about 5×10^{-7} mbar. The magnetic field in the collision region is reduced by two concentric μ-metal shields inside the chamber.

Incident electrons are derived from the hairpin tungsten filament (cathode) by thermo-electronic emission. The electron beam is then extracted and focused into the interaction volume by seven electrodes of the electron gun. Electron energy can vary in the range from 40 to 300 eV and is determined by the potential difference between the filament and the last, grounded, electrode, with energy resolution about 0.5 eV. When the current through the cathode filament was about 2.22 A, the electron current, measured with the Faradays cup without gas in the chamber, was approximately 100 nA. The electron gun can be rotated around the fixed detection system in the angular range from −40° to 126°.

Atomic/molecular beam is formed by stainless-steel gas needle. The length of the needle is l = 40 mm and its diameter, d = 0.5 mm. According to Lucas [40], beam properties can be predicted and optimized. Optimum atomic beam is obtained when $I(0)^2/(NH^2)$, where $I(0)$ is axial intensity, N throughput and H beam halfwidth, is maximum. It is shown that $I(0)^2/(NH^2) \propto l^2/d$ [41]. So, the optimum beam is acquired when the ratio of square of single tube length and its diameter is maximum, which is in our case 3200. These expressions can be employed for tubes where $\gamma = d/l$ (true dimensionless ratio of length and diameter) is below 10 ($\gamma < 10$) and gas pressure is low enough so that the mean free path of a particle is larger or equal than d ($\lambda \geq d$). In our experimental setup γ = 80 and $\lambda \approx d$.

After the interaction with the molecular beam, scattered electrons are entering the detection system. First, they are focused and slowed down to the constant pass energy of the analyzer by the four-electrode lens. Then, they are energy-analyzed by the double cylindrical mirror analyzer (DCMA). After that, elastically scattered electrons are focused by the three-electrode lens into the detector (single channel electron multiplier).

The intensity of elastically scattered electrons from methane molecule is measured as a function of scattering angle, from 25° to 125° (in 5° steps), at given incident electron energy, from 50 to 300 eV (in 50 eV steps). Experimental parameters were adjusted so that the interaction volume was kept constant. Deviations that can occur at small angles are corrected by comparing cross-sections from Ar at given energy with other authors' data [42,43]. During the measurements, working pressure in the chamber was about 4×10^{-6} mbar. For each electron energy, scattering intensities are measured at least three times. To discount background scattering contributions, a gas beam was introduced to the chamber through a side leak, away from the collision area. Scattering intensities are measured and subtracted from apparent signal for each angle.

The obtained relative DCSs are converted to the absolute DCSs using relative flow method (RFM) [44]. Briefly, the signal of scattered electrons from the target molecule is compared with elastically scattered electron intensity from reference gas, at the same scattering angle, for the same electron energy and experimental conditions. The same experimental conditions for both gasses implies that their beam profiles must be closely equal, which is acquired, according to Olander and Kruger [45], under two conditions: the mean free paths (λ) behind the gas needle for both gasses must be the same and the Knudsen number, K_L, defined as λ/l, must be in the appropriate range, $\gamma \leq K_L \leq 10$. The first condition is fulfilled when pressure ratio of test molecule and reference gas is inversely proportional to the ratio of squares of their gas kinetic diameters. In this study, Ar is used as a reference, with its diameter of approximately 3.58 Å. The gas kinetic diameter of the target gas, methane is approximately 3.8 Å, which gives ratio 1.13; almost the same gas pressure behind gas needle for both gasses must be applied. As for the second condition, gas pressures were low enough so that K_L is approximately equal to γ, although some studies have shown that even when K_L is much lower than γ, beam profiles for most gasses can still be very alike [46,47]. Besides scattering intensities of both gasses, relative flow rate is determined by measuring pressure increase in time by admitting gas into the constant volume, while a chamber outlet was closed.

The known absolute DCSs for Ar are taken from Ranković et al. [42] for incident electron energies 50–200 eV and 300 eV and from Williams and Willis [43] for electron energy of 250 eV. In both papers, the absolute values were derived by measurements of angular dependences of elastically scattered electrons using electron spectrometers, two 127° cylindrical electrostatic energy analyzer in [43], and a double cylindrical mirror analyzer in [42] but employing different normalization procedures. While in [42] the relative flow method with He as a reference gas was used, in [43] a phaseshift analysis of the relative angular distributions of electrons elastically scattered in the energy region of the resonances $^2P_{3/2,1/2}$ of Ar, i.e., between 11.0 and 11.4 eV, were used. Nevertheless, the absolute DCS values for Ar agree within mutual uncertainties as discussed in [42]. Since our normalization is based upon relative flow method, we prefer to use values from the most recent paper [42] and only for the energy of 250 eV, which is not available in [42] we used those from [43].

Since our experimental DCSs are obtained in the limited angular range, in order to obtained elastic integral (ICSs) and momentum transfer (MTCSs) cross-sections, our DCSs must be extrapolated to the smallest (0°) and the highest (180°) scattering angles. Our extrapolation takes into account the theoretically obtained shapes of DCSs (present model 2, at small (0–25°) and high (120–180°) scattering angles and present experimental values of DCSs near 25° and 120°. Thereafter, ICSs and MTCSs were obtained using extrapolated DCSs and appropriate integration defined as:

$$ICS = 2\pi \int_{0}^{\pi} DCS(\theta) \sin\theta d\theta \tag{14}$$

$$MTCS = 2\pi \int_{0}^{\pi} DCS(\theta)(1 - \cos\theta) \sin\theta d\theta \tag{15}$$

The uncertainties of the relative DCSs consisted of statistical uncertainties and short-term stability uncertainties, caused by instability of the system. This uncertainty is increased by 20% for small scattering angles, due to the potential alteration of the interaction volume. Dominant uncertainties for absolute DCSs are those from reference cross-sections for Ar [42,43], and are taken to be about 20%. The DCS uncertainties obtained in such a manner, Δ, are presented in parenthesis within Table 2. The total uncertainties for absolute DCSs are about 30% for small angles and about 20% for the rest of the angular range. The total uncertainties of ICSs and MTCs arise from the DCSs uncertainties mentioned above and uncertainties of the extrapolation of DCSs to 0° and to 180° and numerical integration (10%).

4. Results

Measured results of the absolute differential cross-sections, integral cross-sections, and momentum transfer cross-sections, together with their corresponding uncertainties, are shown in Table 2. The results cover six incident electron energies, from 50 eV to 300 eV and angular range from 25° to 125°. In Figure 1, the present theoretical and experimental DCSs for all six incident electron energies are shown graphically. For the sake of comparison, other authors' data [16,23,24,27–31], listed in Table 1, are shown in the same figure.

Theoretical results are shown in two approximations: the simple sum of individual atomic cross-sections (model 1, dashed black line) and with molecular effects taken into account (model 2, solid black line). It can be seen that those effects significantly modify DCSs. One of them, the absorption potential, plays a dominant role in this modification of cross-sections. In comparison with present experiment and other authors' results, theory with included molecular effects showed better agreement, both qualitatively and quantitatively, as expected.

Obtained ICSs, together with other authors' results [17,25,29–31,33,34], are presented in Figure 2.

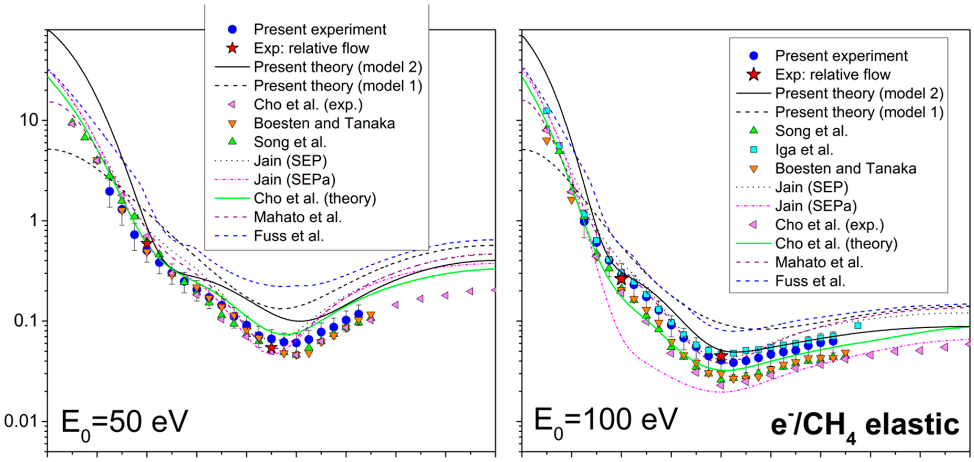


Figure 1. *Cont.*

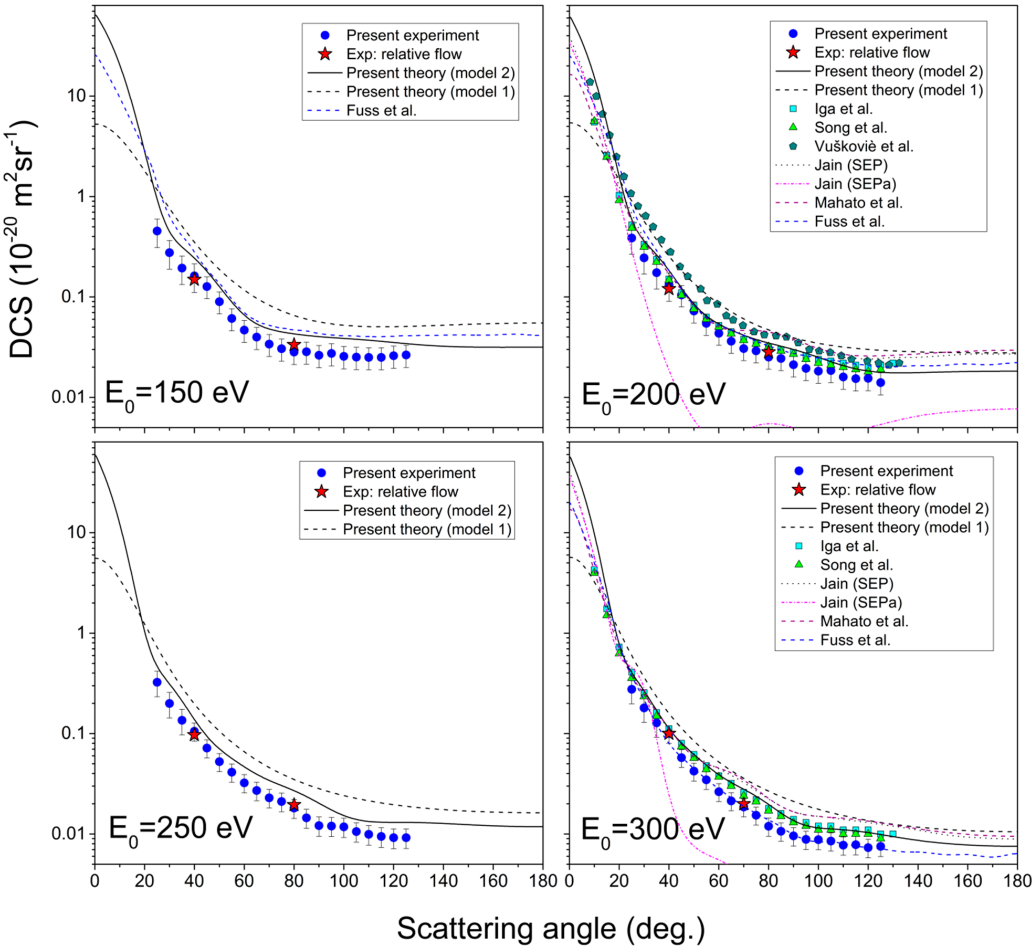


Figure 1. Angle differential cross-sections for elastic electron scattering from methane molecule, for six incident electron energies, from 50 eV to 300 eV. The present results include experiment (blue circles), relative flow absolute data (red stars), theory with molecular effects (full line) and simple sum theory (dashed line). Previous results, tabulated in Table 1, are also shown for the sake of comparison.

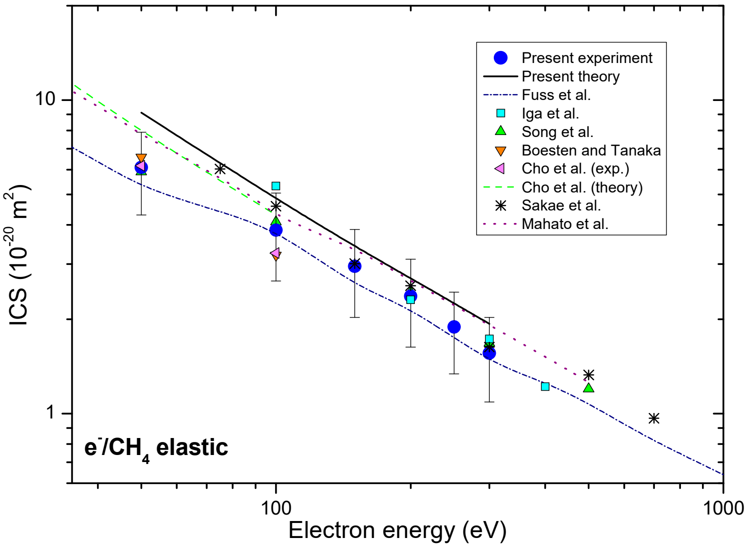


Figure 2. Integral cross-sections for elastic electron-methane collision, presented in energy range from 35 eV to 1000 eV. Present experimental (blue circles) and theoretical (solid black line) results are shown together with previous experimental, as well as the theoretical results, for comparison.

5. Discussion

Experimental DCS at 50 eV exhibits wide minimum at 100° scattering angle, for which position and depth are in good agreement with other authors' results [17,25,29,32,33], especially experimental ones [17,25,29]. Our calculations overestimate the measured DCS, but it matches with shape and is in a good agreement with other theories [29,32] at high scattering angles, above 110°. It is interesting to note that all existing experimental values at 50 eV impact energy agree among themselves within the estimated uncertainties. It is rather a problem with theories, which, in most cases, overestimate absolutes values or do so at certain angular ranges.

There are many experimental and theoretical data for DCS at 100 eV. This cross-section shows a wide and shallow local minimum at 80° scattering angle, which vanishes for incident electron energies above 150 eV. Its position is the same or similar for every shown result. Our measurement and calculation are in strong agreement with the experimental result of Iga et al. [31] and with the theories of Jain (SEP) [32] and Mahato et al. [33], except at higher scattering angles (from 105°). Other results are in good agreement with the shape, but quantitatively are underestimated in comparison with the present result. It seems that there are two classes of experimental values that differ in absolute values, one by Boesten and Tanaka [25] and Cho et al. [29] and the other by Iga et al. [31] and the present measurements. One of the significant differences between these two sets of data lie in the choice of the reference gas, the former used He while the later used Ne and Ar as a reference. Nevertheless the cross-sections for He are known with better accuracy than those of Ne and Ar, it seems plausible to conclude that more similar flow conditions between the reference gas and the target one give more reliable data. If it has been possible to obtain perfectly the same all conditions necessary for applying the relative flow method, then the choice of reference gas would be the one with the best-known cross-sections, i.e., He gas. However, since the method itself introduces additional uncertainties, in our opinion, it would be the best procedure to compare cross-sections with relatively similar flows within gas inlet system.

As for DCSs for 150 eV, there are only results by Fuss et al. [34] available for comparison. At this energy, there are no local minima, like for 50 eV and 100 eV. Instead, there is a wide plateau from 70° scattering angle. Experiment and theory are in good agreement by the shape, but the experiment is, on average, about 30% quantitatively lower.

DCSs for 200 eV (both measured and calculated) show good agreement (within experimental uncertainty) with experimental results of Iga et al. [31], recommended data by Song et al. [17] and theoretical results by Jain (SEP) [32] and Mahato et al. [33] for smaller scattering angles (below 70°). Results by Vušković and Trajm ar [26] are good by shape but higher in absolute value.

For DCS for 250 eV incident electron energy, to the best of our knowledge, there are no published experimental or theoretical results. In the graph, it can be seen that our theory is slightly higher than the measured results, but both are similar qualitatively.

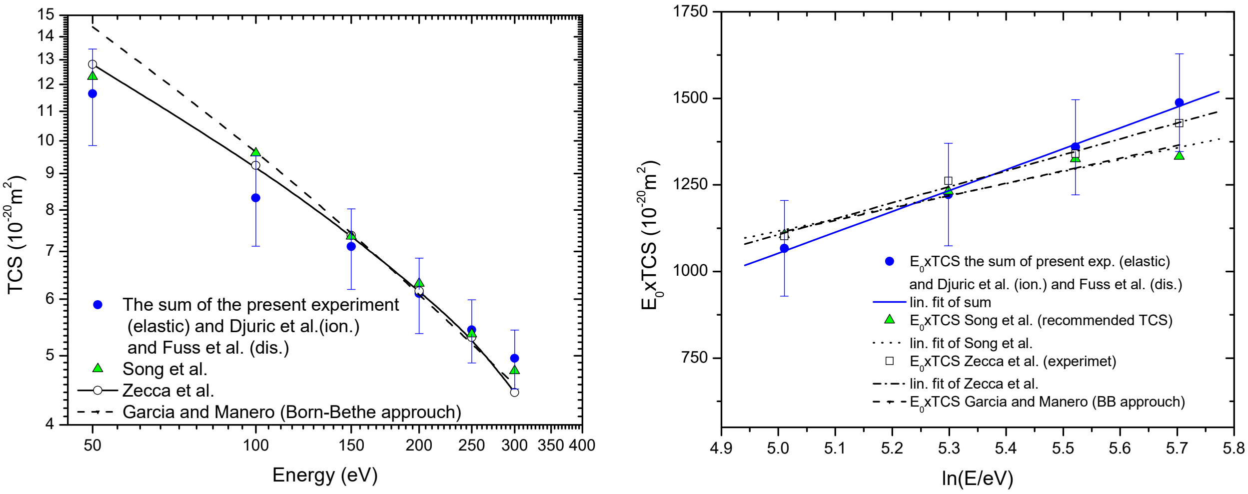
At 300 eV, the shapes and values of present theory and previous results by Iga et al. [31] and Song et al. [17] are in almost perfect agreement. The experimental result is just slightly lower on the absolute scale. Same as for every other energy, calculations by Jain [32] and Mahato et al. [33] agree good for smaller scattering angles, but for higher, they little overestimate other results.

The values of DCSs span over three and four orders of magnitude in presented energy range, what is the characteristic behavior for molecular targets and noticed also in the previous targets [42,48]. The general agreement among different experimental datasets and calculations is very good, and that is what one may expect at the present level of advanced experiments and sophisticated calculations [49].

The present experimental integral cross-sections ICSs are shown in Table 1 and together with other available results in Figure 2. Our experimental ICSs are placed between recommended Fuss et al. [34] and theoretical results Mahato et al. [33]. In the electron energy range from 50 eV to 300 eV most of the other experimental ICSs, like those by

Boesten and Tanaka [25], Sakae et al. [30], Iga et al. [31], Song et al. [17], lie within the same uncertainty limits. Our experimental DCS data are obtained in rather limited angular range, and that is why the presented integral cross-sections depend strongly upon the extrapolation procedure. We have normalized our calculated DCS (model 2) to our measured absolute data to best match in shape and then used these values for integration. These values are presented in Table 2 with the uncertainty of 30% that arises from different plausible extrapolations. The absolute uncertainties of ICS and MTCS values are obtained from the difference of the corridor that is represented by maximal, DCS + $\Delta/2$, and minimal DCS $-$ $\Delta/2$ values.

If total cross-section (TCS) we calculate as the sum of our measured ICSs, and ionization cross-sections obtained by Djurić et al. [50] plus the recommended neutral dissociation cross-sections by Fuss et al. [34], the TCS values obtained in such way agree well, within experimental uncertainties, with previously published experimental values by Zecca et al. [51] and recommended values by Song et al. [17]. Furthermore, for electron energies greater than 150 eV present TCS well agree with the semiempirical TCS by García and Manero [52] extrapolated in the interval energies of this paper. Total cross-sections for electron-methane collision in the energy range from 45 eV to 300 eV are contrasted in Figure 3a, while the corresponding Fano-Bethe plot is shown in Figure 3b. For electron energies from 150 eV to 300 eV Bethe plot of present TCS, References [17,51] and extrapolated semiempirical TCS García and Manero [52], agree within the limits of experimental uncertainties. This, under the given conditions, suggests that Born-Bethe approximation is valid in the electron energy range from 150 eV to 300 eV.



(**a**) (**b**)

Figure 3. Total cross-sections for electron-methane collision in energy range from 45 eV to 300 eV. ●, present; ▲, Song et al. (recommended values) [17]; —○—, Zecca et al. (experiment) [51]; - - -, García and Manero (Born-Bethe approach) [52]; (**a**) Absolute values; (**b**) The Fano-Bethe plot: ———, linear fit of present; • • •, linear fit of Song et al. [17]; –·– linear fit of Zecca et al. [51].

6. Conclusions

In order to provide the insight into methane/electron interaction, measurements and calculations of elastic electron scattering from methane target were performed. To summarize, calculated and measured cross-sections for elastic CH_4-electron scattering in (50–300) eV incident electron energy range are reported and, conceivably, they will serve as a dependable standard for related investigations in the future. Good agreement between present theory and experiment and results available in the literature is noticed. Also, it is shown that molecular effects (especially absorption effects) play a crucial role on calculated cross-sections, particularly for very small scattering angles (below 20°). The experiment was performed in two independent steps. First was measuring relative DCSs for fixed electron energy in function of scattering angle. Second was obtaining pair of absolute points for every energy, by relative flow method and Ar as reference gas. These absolute points were then used for normalization of relative DCSs. These independent results agree well, which is confirmation of the reliability of the experimental method. DCSs for the incident energy 250 eV is given without previous results known to the authors.

Nevertheless there are many studies of electron elastic scattering by methane molecule, our impression is that the present study is important to pinhole the absolute cross-sections, to confirm recommended sets of data for this process given by Song et al. [17] and to bring new results at one impact energy. Last but not the least, we stress the problem of the choice of a reference gas in the relative flow measurements and the necessity of choosing gases with similar flowing conditions. That could bring methane molecule to be a new standard for cross-sections measurements of other hydrocarbons or larger organic molecules.

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Abbreviations

R. F.	radio frequency
PECVD	plasma-enhanced chemical vapor deposition
DCSs	differential cross-sections
ICSs	integral cross-sections
MTCSs	momentum transfer cross-sections
SCAR	screen corrected additivity rule
ELSEPA	Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules
DCMA	double cylindrical mirror analyzer
RFM	relative flow method
TCS	total cross-section

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Article

Absolute Differential Cross-Sections for Elastic Electron Scattering from Sevoflurane Molecule in the Energy Range from 50–300 eV

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Abstract: We report the results of the measurements and calculations of the absolute differential elastic electron scattering cross-sections (DCSs) from sevoflurane molecule ($C_4H_3F_7O$). The experimental absolute DCSs for elastic electron scattering were obtained for the incident electron energies from 50 eV to 300 eV, and for scattering angles from 25° to 125° using a crossed electron/target beams setup and the relative flow technique for calibration to the absolute scale. For the calculations, we have used the IAM-SCAR+I method (independent atom model (IAM) applying the screened additivity rule (SCAR) with interference terms included (I)). The molecular cross-sections were obtained from the atomic data by using the SCAR procedure, incorporating interference term corrections, by summing all the relevant atomic amplitudes, including the phase coefficients. In this approach, we obtain the molecular differential scattering cross-section (DCS), which, integrated over the scattered electron angular range, gives the integral scattering cross-section (ICS). Calculated cross-sections agree very well with experimental results, in the whole energy and angular range.

Keywords: sevoflurane; cross-section; elastic scattering; electrons

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1. Introduction

Sevoflurane (SF) is sweet-smelling non-flammable highly fluorinated methyl isopropyl ether with a boiling point at a temperature of 58.5 °C. Molar mass is 200.055 g/mol, vapor pressure 197 mmHg at 26 °C, and dipole moment 2.33 D [1]. It is one of the most commonly used inhalational anaesthetics, and it has been widely investigated. The recent review on inhaled anaesthetics [2] covered their environmental role, occupational risk, and clinical use. Gaya da Costa and co-authors [2] extensively elaborated on the case of sevoflurane molecule and its contribution to the global warming effect as a volatile anaesthetic (especially in combination with the use with N_2O), pointed out that its threshold has not yet been established in the workplace as waste anaesthetic gas, considering its side effects in a clinical context (epileptiform electroencephalogram patterns in both adults and paediatric populations; the cardio protective effect in patients with coronary artery disease undergoing vascular surgery, kidney transplantation or lung surgery). The atmospheric lifetimes of the halogenated anaesthetics, halothane, enflurane, sevoflurane, isoflurane, and desflurane to the reaction to the hydroxyl radical (OH) and UV photolysis have been determined from observations of OH reaction kinetics and UV absorption spectra [3]. Halothane, enflurane, and isoflurane showed distinct UV absorption in the range 200–350 nm, and no absorption in the wavelength range 200–350 nm was detected for sevoflurane. Tang et al. [1] analysed the effects of general anaesthetics on their potential targets by large-scale molecular simulation. The structural parameters and partial atomic charges of the anaesthetics, considered to be of great importance, were determined. Geometric optimizations using the Hartree–Fock and the B3LYP (Becke, 3-parameter, Lee–Yang–Parr) density functional theory methods with the large 6–311+G (2d,p) basis set were performed to determine the structures and charge distributions of two halogenated anaesthetics; sevoflurane and halothane. Lesarri and co-authors [4] investigated the conformational landscape of the volatile anaesthetic sevoflurane. The structure of the anaesthetic haloether sevoflurane (CH_2F–O–$CH(CF_3)_2$) has been resolved using Fourier-transform microwave (FT-MW) spectroscopy in a supersonic-jet expansion. In isolated conditions, sevoflurane adopts a single conformation characterized by a gauche fluoromethoxy group and a near-symmetric orientation of the isopropyl group with respect to the ether plane (cis H–Cipr–O–CF). A schematic drawing of sevoflurane is shown in Figure 1.

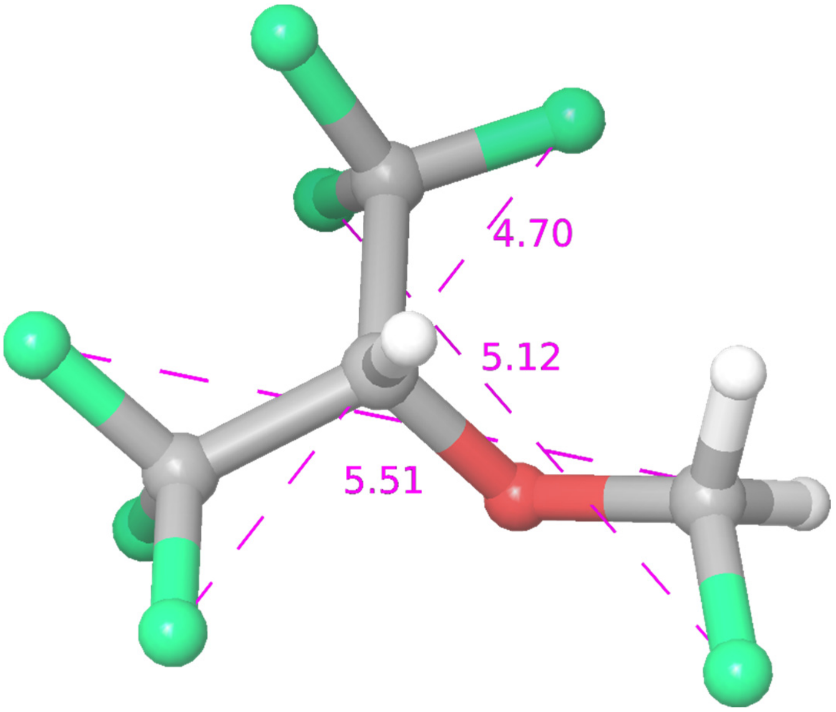

Figure 1. Schematic drawing of sevoflurane.

Don et al. [5] proposed a vibrational assignment of sevoflurane and studied its interaction with the aromatic model compound benzene, using the vibrational spectroscopy of supersonic jet expansions and of cryo solutions in liquid xenon. Sevoflurane has been investigated from the medical point of view also. Shiraishi and Ikeda [6] studied an uptake and biotransformation of sevoflurane in humans and concluded that, despite its relatively large minimum alveolar concentration (MAC), sevoflurane has a small uptake due to its low solubility, but the degradation rate is shown to be high, resulting in a higher serum fluoride concentration than for other halogenated anaesthetics. Most recently, Dong et al. [7] assessed mice and neurons treated with anaesthetics sevoflurane and desflurane, and applied nanobeam-sensor technology, an ultrasensitive method, to measure tau/p-tau amounts. They showed that the sevoflurane induces tau trafficking from neurons to microglia.

Lange et al. [8] have investigated the lowest-lying electronic states of isoflurane and sevoflurane in the 5.0–10.8 eV energy range by experimental and theoretical methods. Photoabsorption spectra of isoflurane and sevoflurane have been measured with synchrotron radiation over the photon range 5.0–10.8 eV. Low-lying excited singlet valence and Rydberg states are investigated, and the assignments supported by quantum chemical calculations, the latter also helping to identify the triplet states. The measured absolute cross-sections have been used to calculate the photolysis lifetimes of isoflurane and sevoflurane in the Earth's atmosphere.

Electron collisions with sevoflurane have also been investigated. Very recently, Lozano et al. [9] reported total scattering cross-section from sevoflurane of 1–300 eV electrons. The experimental results, obtained from an implemented magnetic beam apparatus, are compared with theoretical results from the independent atom model, with a screening corrected additivity rule including interference effects and rotational excitation.

As pointed out by Tanaka et al. [10], the absolute electron-impact excitation cross-sections could be obtained by normalization to elastic scattering cross-section (which is the subject of the present study), or in other ways to determine the binary encounter (BE) scaling curve, after measuring the DCSs at high-energy impact (>100 eV), and for small scattering angles. A comprehensive review of experimental techniques and calculation methods for determination of electron cross-sections from biomolecules, biofuels and their fragments, has been recently given by Brunger [11], covering extensive literature in the field.

In this paper, theoretical and experimental results for elastic electron scattering from sevoflurane, in the medium energy range, are shown, complementing the investigations of electron interaction with this molecule. According to our knowledge, these are the first reported results for absolute differential cross-sections in the energy range from 50–300 eV.

Experimentally obtained data include absolute differential cross-sections for elastic electron scattering for the incident electron energy range from 50 to 300 eV (with 50 eV steps) and an angular range from 25° to 125° (with 5° steps), and integral and momentum transfer cross-sections for every measured energy. The experiment was performed on a crossed-beam apparatus. Relative points were put on the absolute scale with the help of the relative flow method, using Ar as a reference gas. Theoretical results are obtained using the IAM-SCAR+I method (independent atom model (IAM) applying the screened additivity rule (SCAR) with interferences terms included (I)). A very good level of agreement has been found between the present experimental and theoretical data, within the experimental uncertainties.

The paper is organized as follows. The experimental setup and measurement procedure are given in Section 2. The theory and calculations of DCSs are explained in Section 3. Obtained results are shown graphically and in the table, and discussion is shown in Section 4. Section 5 is reserved for the conclusion.

2. Experiment

A schematic drawing of the experimental set-up is shown in Figure 2. Our beam profile has been determined in a previous set of measurements [12–14]. In our experiment, the source of molecular beam is a stainless steel gas needle, with a diameter of $d = 0.5$ mm and a tube length of $l = 40$ mm, which gives the ratio $\Gamma = d/l = 80$, while the input pressures were such that the free mean path (λ) was larger than the inner diameter of the tube. According to Lucas [15], the proposed conditions for Γ and λ are $\Gamma > 10$ and $\lambda \approx d$, so we fulfil all the requirements for the well-collimated beam, and the derived expressions can be used in our experiment. Moreover, author [15] states that the beam properties will be optimized if the ratio of the square of single tube length and its diameter is maximized, which, in our case, is 3200.

The analysing system consists of a front four-electrode lens, energy analyser, and rear three-electrode lens. The four-electrode lens is used for collecting, directing, and focusing scattered electrons to the energy analyser after slowing them down to the constant analyser pass energy. Electron energy analyser is a double cylindrical mirror analyser (DCMA), which, essentially, represents two cylindrical analysers connected in series. Pass energy is determined by the potential difference between the cylinders. The three-electrode lens is used for focusing analysed electrons into the detector (single channel electron multiplier).

Since detecting particles are electrons, detector entrance is grounded, and exit is on a high positive potential.

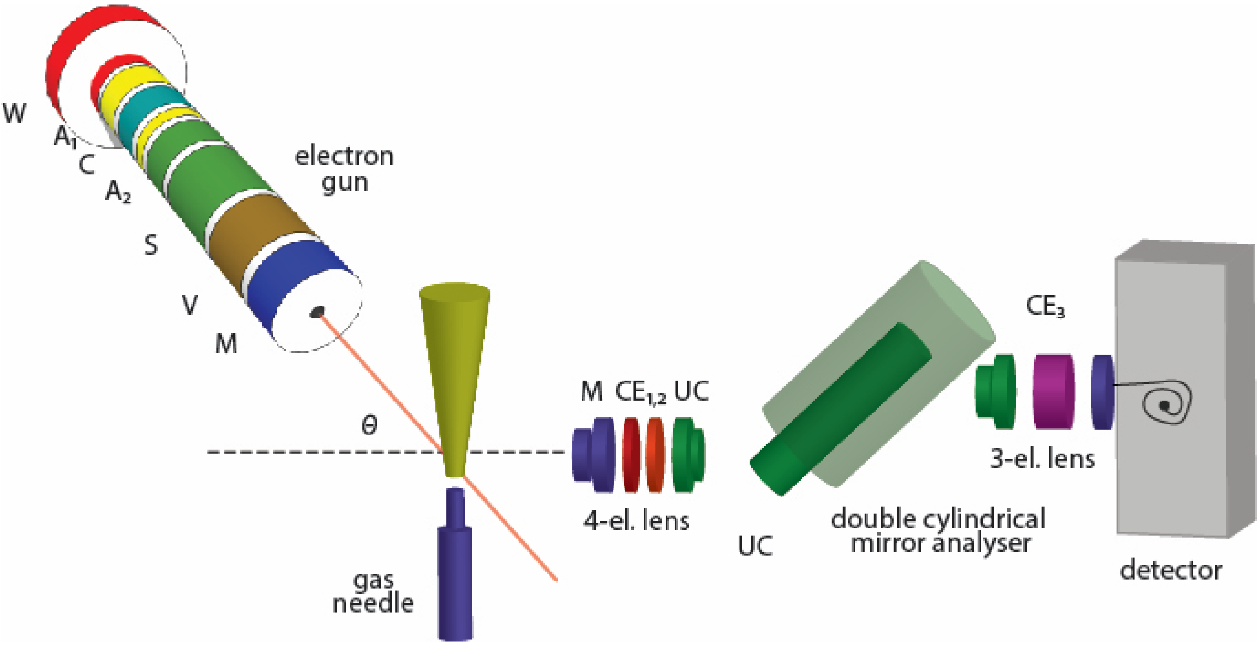

Figure 2. Schematic drawing of the experimental set-up.

The anhydrous sevoflurane ($C_4H_3F_7O$) used in this experiment had a declared purity better than 99%. Before starting the measurements a few freeze-thaw-pump cycles under vacuum have been made. Sevoflurane (SF) is a liquid at room temperature and was introduced into the scattering region from a glass container via a gas line system. SF molecule is characterized by vapor pressure (197 mm Hg at 26 °C) and relatively high dipole moment (2.33 D). Therefore, to provide stable experimental conditions, everything was heated to approximately 50 °C during the gas phase measurements in analogy with previously studied molecular targets [16,17]. In the present work, pipes and the needle were also heated providing a stable driving pressure behind the needle and also for avoiding the absorption effects [18].

In order to reduce magnetic disturbance, the experimental setup is placed in the chamber shielded by the two concentric μ-metal layers. The pre-experimental pressure in the chamber was about $5 \cdot \times 10^{-7}$ mbar and the working pressure was an order of magnitude higher.

The experimental procedure for acquiring the absolute differential cross-sections for elastic scattering of electrons from sevoflurane molecule consists of two main stages:

- Stage 1: obtaining relative DCSs by measuring the intensity of electrons elastically scattered from SF, in the function of scattering angle (from 25° to 125° in 5° steps), for a given incident electron energy (50, 100, 150, 200, 250 and 300 eV). Electron intensities are measured at least three times for every incident energy. Background contributions are suppressed by introducing gas into the chamber, away from the interaction volume, via a side leak, and by subtracting measured intensities from the apparent signal for every angle at the given energy;
- Stage 2: Obtaining absolute points (two) for every electron energy, and normalizing relative DCSs on them. Absolute points are obtained using the relative flow method [19,20].

In the present work, DCSs for elastic electron scattering from sevoflurane have been measured at selected incident electron energies, from 50 to 300 eV (in 50 eV steps), and at scattering angles from 20° to 125° (in 5° steps). At given electron energy, the relative cross-section has been derived as a function of scattering angle by measuring the elastic scattering intensity at the maximum of the elastic peak. The background contributions of the elastic electron intensities, which were around 10% at higher energies, were subtracted from the measured electron yields. It should be noted that the background contributions were generally more important at low incident energies and scattering angles (around 15%). During the measurements, potentials on electron gun electrodes and DCMA were adjusted to keep interaction volume constant. Deviations that can occur at small angles are corrected by comparing cross-sections from Ar at given energy with other authors' data [14,21].

Measured relative DCSs were normalized to the absolute scale according to the absolute points (at 40°, 80°, 90° or 100°), obtained by a Relative flow method (RFM) previously explained in detail [22]. In RFM we compare intensities of elastically scattered electrons on the target molecule (SF) and referent gas (we used Ar), under the same experimental conditions [19,20]. In order to obtain the same experimental conditions, the same beam profiles, for both target molecule and referent gas must be provided. According to Olander and Kruger [23], the same beam profiles can be obtained with two conditions: (1) the mean free paths for both gases must the same and (2) the mean free path is approximately equal to the diameter of stainless steel gas needle. $\lambda \approx d$. In the experiment, the first condition is achieved by adjusting pressures behind the gas needle inversely proportional to the ratio of the squared gas kinetic diameters, and for second condition gas pressures need to be low, which is fulfilled in our experiment [14]. Gas kinetic diameter for Ar is 3.58 Å and for sevoflurane 5.51 Å, so the pressure ratio was P_{Ar}: P_{SF} = D^2_{SF}: D^2_{Ar} ~ 2.4. When the same beam profiles for both, target molecule (DCS_x) and referent gas (DCS_{ref}) are obtained, according to Nickel at al [19,20], absolute differential cross-sections for target molecule $DCSx$ (E, θ) can be calculated, knowing absolute differential cross-sections for the referent gas DCS_{ref} (E, θ), at the same energy and angle, using a formula:

$$DCS_x(E,\theta) = DCS_{ref}(E,\theta)\frac{N_x F_{ref}}{N_{ref} F_x}\sqrt{\frac{M_{ref}}{M_x}} \tag{1}$$

Quantities that we measure in the experiment are: Flow rate (F) and intensity of elastically scattered electrons (N). M_{ref} and M_x are molecular masses for referent gas and target molecule, respectively. The relative flow rate has been determined by closing an outlet to the chamber, admitting target gases into a closed constant volume, and then measuring the pressure increase in time. The flow is determined from the experimental curve of pressure versus time fitted by the least-squares method. The whole system was heated to minimize absorption effects [18], which can influence measuring flow rates and determining the flow.

Our experimental spectrometer UGRA is limited in performing angular dependent differential cross-sections measurements (25–125°) and to obtain integral (*ICSs*) and momentum transfer cross-sections (*MTCSs*) we need to extrapolate measured *DCSs* to 0° and 180°. For extrapolation, from 0–25°, and 125–180° we used calculated results obtained by IAM + SCAR + I procedure (see section Theory) and appropriate integration. Our experimental *DCS* data are obtained in a rather limited angular range and that is why the presented integral cross-sections depend strongly upon the extrapolation procedure. The exact formulae used for the integration are in the form:

$$ICS = 2\pi \int_0^{\pi} DCS(\theta)\sin\theta d\theta \tag{2}$$

$$MTCS = 2\pi \int_0^{\pi} DCS(\theta)(1-\cos\theta)\sin\theta d\theta \tag{3}$$

The uncertainties of the relative *DCSs* consist of statistical uncertainties and short-term stability uncertainties, caused by the instability of the system. This uncertainty is increased by 20% for small scattering angles, due to the potential alteration of the interaction volume. Dominant uncertainty for absolute *DCSs* are those from reference cross-sections for Ar [14,21], and are taken to be about 20%. The total uncertainties, derived as the square root of the sum of squares of individual independent uncertainties, for absolute *DCSs* are about 30% for small angles and about 22% for the rest of the angular range. The total uncertainties of *ICSs* and *MTCs* arise from the *DCSs* uncertainties mentioned above and uncertainties of the extrapolation of *DCSs* to 0° and 180° and numerical integration and were approximately 30%.

3. Theory

To calculate the differential elastic, integral elastic, and inelastic as well as the total cross-sections we have used the IAM-SCAR+I method (independent atom model (IAM) applying the screened additivity rule (SCAR) with interferences terms included (I)). This method has been described in detail in previous publications [9,24–28]. Briefly, the molecular target is described as an aggregate of its individual atoms (i.e., C, H, F, and O in this case). Each atomic target is represented by an ab initio interacting complex optical potential given by:

$$V_{opt}(\vec{r}) = V_R(\vec{r}) + iV_{abs}(\vec{r}) \tag{4}$$

In Equation (4), the real part accounts for elastic scattering while the imaginary part represents the inelastic processes which are considered as the 'absorption part' following the procedure of Staszewska et al. [29]. The real part is divided into three terms that include:

$$V_R(\vec{r}) = V_s(\vec{r}) + V_{ex}(\vec{r}) + V_{pol}(\vec{r}), \tag{5}$$

where vs. represents a static term derived from a Hartree-Fock calculation of the atomic charge distribution [30], V_{ex} an exchange term to account for the indistinguishability of the incident and target electrons [31], and V_{pol} a long-range polarization term [32].

The molecular cross-sections are obtained from the atomic data by using the screening corrected additivity rule (SCAR) procedure [33], incorporating interference (I) term corrections [25], by summing all the relevant atomic amplitudes, including the phase coefficients. In this approach, we obtain the molecular differential scattering cross-section (DCS), which integrated over all the scattered electron angular range gives the integral scattering cross-section (ICS). Moreover, by taking the sum of the ICS for all open channels (elastic ICS and inelastic ICS) the total cross-section (TCS) could be obtained. Note that we do not include at this stage any contribution from vibrational and rotational excitation processes.

Sevoflurane is a polar molecule with a permanent dipole moment of 2.22 D [1] and therefore rotational excitations, not accounted for by the above procedure, are relevant within the scattering scheme. In order to approximately include differential and integral rotational excitation cross-section in the present study, we used the first-Born approximation, following the procedure described in [27]. In these conditions, these cross-sections can easily be calculated by considering the molecule as a rigid rotor, with the initial rotational excited state distribution in equilibrium at 300 K, and calculating all the transitions ΔJ = ±1 (J being the rotational quantum number) assuming the Born approximation but including the correction for the larger angles given by Dickinson (see ref. [34] and references therein).

4. Results

Experimental results for DCSs, together with experimental ICSs and MTCSs, for elastic electron scattering from sevoflurane, are presented in Table 1, all with corresponding absolute uncertainties. Experimentally measured and theoretically calculated DCSs are shown graphically in Figure 3. The experiment covers six energies of impact electrons, from 50 eV to 300 eV, and the angular range from 25° to 125° (theory covers all angles, from 0° to 180°). Absolute uncertainties are about 22%, except for small angles, where uncertainties are increased to about 30% due to the potential interaction volume alterations.

Table 1. Experimental results for absolute differential cross-sections (DCSs), integral cross-sections (ICSs) and momentum transfer cross-sections (MTCSs) for elastic electron scattering from sevoflurane. In parentheses are given absolute uncertainties of the last two digits.

θ (°)	DCS (10^{-20} m^2 sr^{-1})					
	50 (eV)	**100 (eV)**	**150 (eV)**	**200 (eV)**	**250 (eV)**	**300 (eV)**
25	3.6(1.1)	2.55(76)	1.50(39)	2.25(74)	1.82(56)	1.53(45)
30	3.07(93)	1.98(59)	1.25(32)	1.44(48)	1.20(37)	1.12(33)
35	2.17(66)	1.64(49)	0.82(21)	1.01(33)	0.99(30)	0.96(28)
40	1.89(43)	1.14(34)	0.69(14)	0.80(26)	0.84(26)	0.72(21)
45	1.77(40)	0.78(23)	0.55(11)	0.71(24)	0.67(16)	0.43(13)
50	1.57(36)	0.61(14)	0.476(94)	0.61(16)	0.43(10)	0.304(66)
55	1.31(30)	0.49(11)	0.386(77)	0.41(11)	0.282(67)	0.235(51)
60	1.01(23)	0.428(98)	0.289(57)	0.270(71)	0.223(53)	0.202(44)
65	0.82(18)	0.369(84)	0.211(42)	0.214(57)	0.220(52)	0.180(39)
70	0.68(15)	0.307(70)	0.155(31)	0.194(51)	0.189(45)	0.160(35)
75	0.55(13)	0.243(56)	0.126(25)	0.195(51)	0.162(38)	0.141(31)
80	0.47(11)	0.203(47)	0.117(23)	0.179(47)	0.150(36)	0.122(27)
85	0.380(86)	0.165(38)	0.127(25)	0.165(44)	0.139(33)	0.107(24)
90	0.339(77)	0.157(36)	0.125(25)	0.160(43)	0.127(30)	0.095(21)
95	0.327(74)	0.154(35)	0.129(26)	0.162(44)	0.117(28)	0.096(21)
100	0.347(79)	0.175(40)	0.128(25)	0.167(44)	0.109(26)	0.091(20)
105	0.396(90)	0.188(43)	0.130(26)	0.160(42)	0.111(27)	0.090(21)
110	0.48(11)	0.225(51)	0.146(29)	0.160(42)	0.118(28)	0.093(20)
115	0.59(13)	0.265(61)	0.161(32)	0.165(44)	0.113(27)	0.089(20)
120	0.71(16)	0.311(71)	0.179(35)	0.173(46)	0.116(28)	0.088(20)
125	0.85(19)	0.367(84)	0.193(38)	0.170(45)	0.122(29)	0.085(19)
ICS's	37(10)	26.9(8.3)	20.5(5.6)	18.8(6.4)	16.6(5.2)	15.3(4.6)
MTCS's	13.5(4.3)	5.8(1.5)	2.94(68)	2.90(85)	2.14(58)	1.66(43)

DCSs have characteristic behavior for molecular targets, noticed previously [12,13]. At 50 eV and 100 eV DCSs exhibit a wide minimum at 100° scattering angle, which disappears at higher incident electron energies. Experiment and theory are generally in good agreement, both in shape and on the absolute scale. There are systematic discrepancies at small angles for all electron energies, probably because of the instability of interaction volume at those angles during the experiment. Also, there are obvious declinations of DCSs for 150 eV electron energies at high scattering angles.

Concerning the normalization procedure of our results, in the relative flow measurements, absolute DCSs for Ar are taken from Ranković et al. [14] for incident electron energies 50–200 eV and 300 eV and from Williams and Willis [22] for electron energy of 250 eV. In both papers, the absolute values were derived by measurements of angular dependences of elastically scattered electrons using electron spectrometers, two 127° cylindrical electrostatic energy analysers in [21], and a double cylindrical mirror analyser (DCMA) in [14]. Authors had different normalization procedures. Ranković et al. [14] used He as a reference gas and Williams and Willis [21] a phaseshift analysis of the relative angular distributions of electrons elastically scattered in the energy region of the resonances $^2P_{3/2.1/2}$ of Ar. Both absolute differential cross-sections agree within mutual uncertainties as discussed in [10]. Since our normalization is based upon RFM, we prefer to use values from the most recent paper [14] because they were obtained at the same electron spectrometer UGRA and only for the energy of 250 eV, which is not available from our apparatus [14], we used those from Williams and Willis [21].

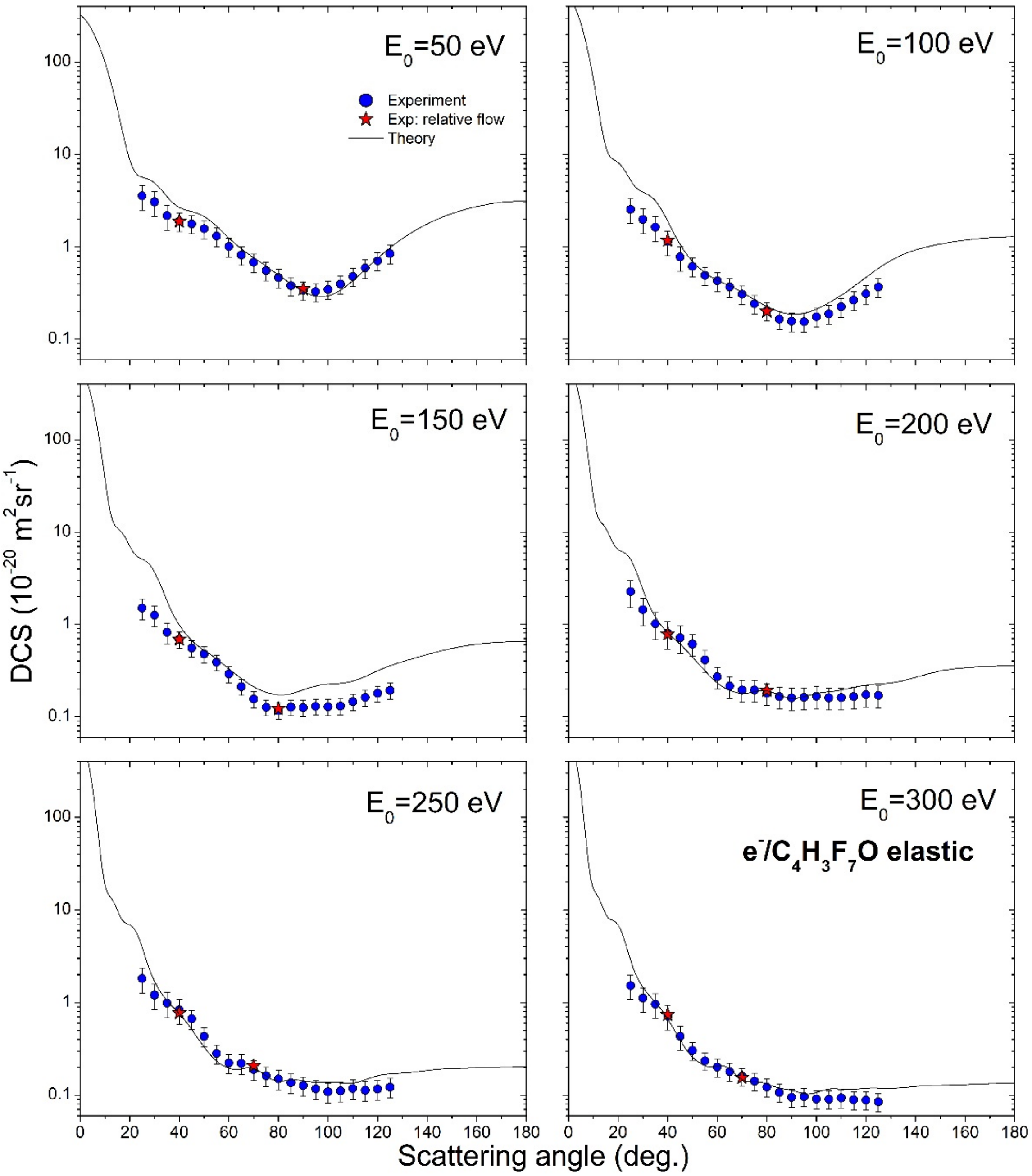

Figure 3. Angularly dependent differential cross-sections for elastic electron scattering from sevoflurane molecule, for six incident electron energies, from 50 eV to 300 eV. The present results include: experiment (blue circles), relative flow absolute data (red stars) and theory (full line).

The shapes of the experimental and theoretical cross-section plots are in excellent agreement, but measured points are 25% lower than the calculated ones. Because our experiment is angularly limited, ICS depends on the used extrapolation method, which is consisted of the normalization of our theoretical DCSs to our measured absolute ones. We have normalized calculated DCS to the measured absolute data to best match in shape and then used these values for integration. These values are presented in Table 1 with an uncertainty of 30% that arises from different plausible extrapolations. The absolute uncertainties of ICS and MTCS values are obtained from the difference of the corridor that is represented by maximal, DCS + $\Delta/2$, and minimal DCS $-$ $\Delta/2$ values.

Measured and calculated absolute differential and integral cross-sections are graphically presented in Figures 3 and 4, and to the best of the authors knowledge, there are no other published results, neither experimental nor theoretical, for DCS or ICSs for elastic electron scattering from sevoflurane in this energy and angular range.

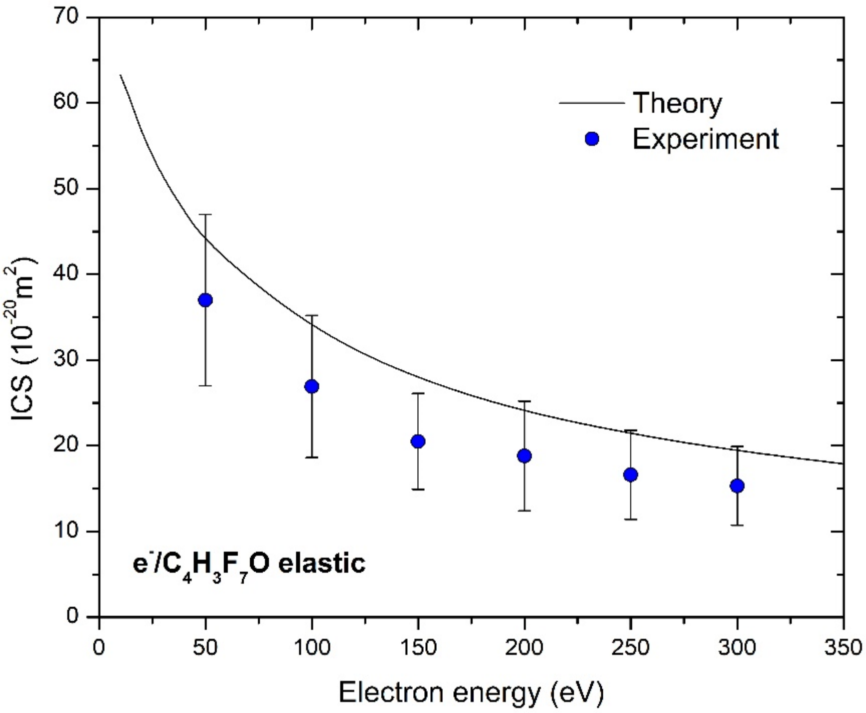

Figure 4. Integral cross-section for elastic electron collision with sevoflurane molecule in the energy range from 10 eV to 350 eV. Experiment (blue circles) and theory (solid black line) are presented.

5. Conclusions

We performed the experimental and theoretical investigation of elastic electron collisions on sevoflurane molecule at intermediate incident electron energies in order to provide insight into electron/sevoflurane interaction. Two independent sets of measurements, relative differential cross-sections at fixed energy in the function of scattering angle and absolute differential cross-sections obtained by relative flow method were performed. The last one provides us with two absolute points for every incident energy, which were used for the normalization to the absolute scale. These two independent sets of measurements showed good agreement which gives reliability to our experimental procedure. We have shown good agreement between the present experiment and theory (IAM-SCAR+I method) on the absolute scale and also in the shape. Using Ar we stress the problem of the choice of the reference gas in the relative flow measurements, since conditions should be provided for the widths (shapes) of the target beam and the reference gas beam to be approximately the same, which is easier to achieve with Ar in relation to He or Ne, since they are much lighter. The importance of this investigation is that according to our knowledge these are the first reported results for absolute differential and integral cross-sections for elastic electron scattering on sevoflurane in the energy range from (50–300) eV.

Author Contributions: Conceptualization, all authors; methodology, J.B.M. and B.P.M.; software, F.B. and G.G.; validation, all authors; experimental investigation, J.V. and J.B.M.; resources, B.P.M.; data curation, B.P.M.; writing—original draft preparation, J.V., J.B.M. and G.G.; writing—review and editing, B.P.M. and J.V.; visualization, J.V. and B.P.; supervision, B.P.M.; project administration, B.P.M.; funding acquisition, B.P.M. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

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Subject **Invitation for topical lecture at CEPAS conference**
From CEPAS Organising committee <cepas@neon.dpp.fmph.uniba.sk>
To <jelenam@ipb.ac.rs>
Date 2013-11-17 20:39

Dear Dear Jelena,

I write you as chairman of the Local Organising Committee of the Conference on Elementary Processes in Atomic Systems - CEPAS. CEPAS is triennial conference and the 6th continuation will be held in Bratislava from 9th to 12th July 2014.

The main topics of the conference are:

photo-processes and laser collisions
electron(positron)/atom collisions
collisions with biomolecules
heavy particles (ion/atom) collisions
interactions with surfaces
processes with nano-sized complex systems

You have been selected by the members of the International Scientific Committee of the CEPAS conference as topical speaker on the topic:

Absolute differential cross sections for elastic scattering

In the program of the conference are planned 6 invited and 24 topical lectures.

It would we for me great honour if you could accept this invitation.
Please let me know your decision.

Yours sincerely,

Stefan Matejcik
Chair of the LOC

Tuesday, 8th July 2014	
15:00 – 19:15	*Registration*
19:30 – 22:00	*Welcome Reception*
22:00	*2014 FIFA World Cup Brazil, 1st Semifinal Match*

Wednesday, 9th July 2014	
8:00 – 8:45	*Registration*
8:45 – 9:00	*Opening*
	Chairman: ***To be announced***
9:00 – 9:45	**Paul Scheier** University Innsbruck, AUT DECORATION OF FULLERENE IONS WITH SIMPLE MOLECULES
9:45 – 10:10	**Oliver Ochedowski** Universität Duisburg-Essen, DEU SWIFT HEAVY ION IRRADIATION OF GRAPHENE
10:10 – 10:40	*Coffee Break*
	Chairman: ***To be announced***
10:40 – 11:25	**John Tanis** Western Michigan University, USA TRANSMISSION OF ELECTRONS THROUGH MICROMETER GLASS CAPILLARIES AND DIFFERENCES WITH IONS
11:25 – 11:50	**Gyula Nagy** Hungarian Academy of Sciences, HUN GUIDING OF MEV ION BEAMS
12:50 – 12:15	**Michael Schulz** Missouri University of Science & Technology, USA MANIPULATING ATOMIC FRAGMENTATION PROCESSES BY CONTROLLING THE PROJECTILE COHERENCE
15:15 – 14:00	*Lunch*
	Chairman: ***To be announced***
14:00 – 14:25	**Roman Čurík** Academy of Sciences of the Czech Republic, CZE INDIRECT DISSOCIATIVE RECOMBINATION OF SIMPLE IONS
14:25 – 14:50	**Masamitsu Hoshino** Sophia University, JPN ELASTIC SCATTERING FROM PLASMA MOLECULES AND RADICALS
14:50 – 15:15	**Peter Papp** Comenius University, SVK ELECTRON IONISATION AND ELECTRON ATTACHMENT OF METALORGANIC COMPOUNDS
15:15 – 15:40	**Pierre-Michel Hillenbrand** GSI Darmstadt, DEU MEASUREMENTS OF RADIATIVE ELECTRON CAPTURE TO THE CONTINUUM (RECC)
15:40 – 16:15	*Coffee Break*
16:15 – 19:00	Poster Session I (max. A1 portrait paper size)
19:00 – 22:00	*Individual Dinner in the City*
22:00	*2014 FIFA World Cup Brazil, 2nd Semifinal Match*

Thursday, 10th July 2014

	Chairman: ***To be announced***
9:00 – 9:45	**Dragana Marić** University of Belgrade, SRB ATOMIC AND MOLECULAR PROCESSES OF INTEREST FOR MODELING OF DISCHARGES IN LIQUIDS
9:45 – 10:10	**Kinga Kutasi** Hungarian Academy of Sciences, HUN SURFACE AND GAS PHASE PROCESSES IN AFTERGLOW PLASMAS AIMED FOR MEDICAL STERILIZATION
10:10 – 10:40	*Coffee Break*
	Chairman: ***To be announced***
10:40 – 11:25	**Don Madison** Missouri University of Science & Technology, USA ACCURACY OF THEORETICAL CALCULATIONS FOR ELECTRON-IMPACT IONIZATION OF MOLECULE
11:25 – 11:50	**Jeff Shinpaugh** East Carolina University, USA ATOMIC COLLISION PROCESSES IN BIOLOGICAL AND CHEMICAL SYSTEMS
12:50 – 12:15	**Sadia Bari** European XFEL GmbH, DEU DISSOCIATION OF PEPTIDES BY IONS AND PHOTONS
15:15 – 14:00	*Lunch*
	Chairman: ***To be announced***
14:00 – 14:25	**Oddur Ingólfsson** University of Iceland, ISL METASTABLE FREGMANTATION OF BIOMOLECULES
14:25 – 14:50	**Jelena Maljković** University of Belgrade, SRB ABSOLUTE CROSS SECTIONS FOR ELASTIC ELECTRON SCATTERING FROM FURAN AND THF MOLECULES
14:50 – 15:15	**Filipe Ferreira da Silva** Universidade Nova de Lisboa, PRT ON ELECTRON INDUCED PROCESSES IN BIOMOLECULES
15:15 – 15:40	**Lothar Schmidt** Goethe-Universität Frankfurt am Main, DEU MOMENTUM TRANSFER TO A FREE FLOATING DOUBLE SLIT: REALIZATION OF A THOUGHT EXPERIMENT FROM THE EINSTEIN-BOHR DEBATES
15:40 – 16:15	*Coffee Break*
16:15 – 16:40	**Martin Čížek** Charles University in Prague, CZE LOW ENERGY REACTIVE COLLISIONS IN O^- + H2
16:40 – 17:05	**Yuri Kozhedub** St. Petersburg State University, RUS ELECTRONIC DYNAMICS IN LOW-ENERGY HEAVY-ION COLLISIONS
19:00	*Conference Dinner – Hotel Borik*

Friday, 11th July 2014

	Chairman: ***To be announced***
9:00 – 9:45	**Yasuyuki Nagashima** Tokyo University of Science, JPN NEW DEVELOPMENTS OF THE PS- STUDIES
9:45 – 10:10	**Tom Kirchner** York University, CAN INTERACTION OF ANTIPROTONS AND PROTONS WITH ATOMS: A DENSITY-FUNCTIONAL THEORY PERSPECTIVE
10:10 – 10:40	*Coffee Break*
	Chairman: ***To be announced***
10:40 – 11:25	**Fernando Martin** Universidad Autonoma de Madrid, ESP ELECTRON AND NUCLEAR DYNAMICS IN THE PHOTOIONIZATION OF MOLECULES
11:25 – 11:50	**Elisabeth Gruber** Vienna University of Technology, AUT TRANSMISSION OF SLOW HIGHLY CHARGED IONS THROUGH 1 NM THICK CARBON NANOMEMBRANES
12:50 – 12:15	**Zoltan Juhasz** ATOMKI, HUN GUIDED TRANSMISSION OF IONS THROUGH NANOCAPILLARIES: VARIATIONS IN DISCHARGING DYNAMICS
15:15 – 14:00	*Lunch*
	Chairman: ***To be announced***
14:00 – 14:25	**Stefan Fritzsche** Helmholtz-Institute Jena, DEU THEORETICAL DESCRIPTION OF RELATIVISTIC ATOMIC COLLISIONS
14:25 – 14:50	**Alexey Verkhovtsev** Goethe University, DEU PHOTOIONIZATION OF FULLERENES AND OTHER NANOCARBON SYSTEMS
14:50 – 15:15	**Sandor Borbely** Babes-Bolyai University SPATIAL INTERFERENCE EFFECTS DURING THE IONIZATION OF ATOMS BY FEW-CYCLE LASER PULSES
15:15 – 15:40	**Florian Trinter** Goethe-Universitaet Frankfurt am Main, DEU TIME DEPENDENCE OF INTERATOMIC COULOMBIC DECAY
15:40 – 16:15	*Coffee Break*
16:15 – 19:00	Poster Session II (max. A1 portrait paper size)
19:00	*Individual Dinner in the City*

Saturday, 12th July 2014

8:30 – 16:00	*Excursion to Chateau Topolčianky and European Bison Park*

Transport of electrons through a long metallic microcapillary: characterization of the outgoing low-energy electron beam

Aleksandar R. Milosavljević [1,*], Jelena B. Maljković [1], Réka J. Bereczky [2], Miloš Lj. Ranković [1],
Bratislav P. Marinković [1] and Károly Tőkési [2]

(1) Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
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The guiding of charged particles – highly charged ions – by insulating nanocapillaries has been firstly reported in 2002 [1] and has been attracting a large attention since then, partly due to potential applications in ion transport [2]. The pioneering work on electron guiding through insulating capillaries has been reported recently [3,4] and the electron guiding phenomena has been discussed in detailed nowadays [5,6]. The aim of the present research is to investigate the electron transport by metallic high-aspect ratio capillaries and their potential use for a robust, spatially well-determined, low-energy electron source, which can be efficiently applied to study electron driven molecular processes under different environmental conditions.

In this work we have investigated transmission of 150 eV incident electrons through a single stainless steel microcapillary (0.9 mm diameter and 19.5 mm length – the aspect ratio of about 22). The intensity of the outgoing electron current has been measured as a function of both the incident beam angle with respect to the capillary axis (tilt angle) and the kinetic energy of outgoing electrons. The "quasi-monochromatic" incident electron beam produces a wide distribution of outgoing electrons, spanning down to practically 0 eV. At large tilt angles (when the direct beam is suppressed due to the close collision with the inner wall of the capillary) this distribution is determined by elastic electron scattering, inelastic processes and secondary electron production. It is, however, interesting that the dependence on the tilt angle changes with the outgoing kinetic energy, and low-energy electrons may dominate at larger tilt angles.

Acknowledgement: The work was supported by the MESTD RS (Project No. 171020), by the Hungarian SRF OTKA No. NN 103279, and by the Bilateral Cooperation Program between the Hungarian and Serbian Academies.

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[2] T. Ikeda et al., *J. Phys. Conf. Series* **399** (2012) 012007.
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[4] S. Das et al., *Phys. Rev. A* **76** (2007) 042716.
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PROGRAMME

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ÚJ SZÉCHENYI TERV

MAGYARORSZÁG MEGÚJUL

A projekt az Európai Unió támogatásával, az Európai Szociális Alap társfinanszírozásával valósul meg.

Organisers acknowledge the support of the TÁMOP-4.2.2.A-11/1/KONV-2012-0036 project implemented through the New Hungary Development Plan and co-financed by the European Social Fund.

Electron transmission through a metallic capillary

J. B. Maljković[1], M. Lj Ranković[1], R. J. Bereczky[2], B. P. Marinković[1], K. Tőkési[2], A. R. Milosavljević[1]

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jelenam@ipb.ac.rs

We present the preliminary experimental results about electron transmission through a single metallic capillary, following our previous investigation of electron guiding through insulating nanocapillaries [1]. The incident electron energy was 150 eV and the aspect ratio of the capillary was 21.67 (length L=19.51 mm and inner diameter d=0.15 mm). The kinetic energy distribution of transmitted electrons was recorded at a tilt angle (the angle between the incident electron beam and the capillary axis) of 2°. The results are obtained by an electron spectrometer, consisted of an electron gun, a double cylindrical mirror energy analyzer (DCMA) and a channeltron detector. Fig. 1 presents the kinetic energy distribution of electrons escaping the capillary. Except the dominant peak, corresponding to the direct beam and the elastic surface scattering, there is a strong fraction of electrons that suffer inelastic collisions and secondary electrons.

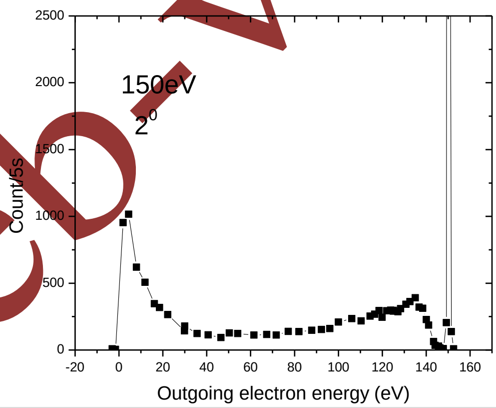

Figure 1. Energy spectrum of the electrons escaping the metalic capillary at the tilt angle 2°.

Acknowledgements: This work was supported by the Bilateral Co-operation Program between the Hungarian and Serbian Academies through project Interactions of charge particles with single insulating capillaries, by the Hungarian Research fund OTKA No. NN103279, Serbian Research Project OI 171020 and by the COST Action CM1204 (XLIC).

References

[1] A. R. Milosavljević et al., *Phys. Rev.* A (2007) 75, 030901(R).

SPIG 2014

27th Summer School and
International Symposium on
the Physics of Ionized Gases

August 26-29, 2014, Belgrade, Serbia

Dr Jelena Maljković

Institute of Physics Belgrade,
University of Belgrade,
Pregrevica 118,
11080 Belgrade
Serbia

Belgrade, 21th October 2013

Dear Dr Maljković,

On behalf of the Scientific and Organizing Committees, we have a pleasure to invite you to attend the *27th Summer School and International Symposium on the Physics of Ionized Gases* (SPIG 2014) and present a **progress report** (20 min, including questions and discussions) aimed at the topics covered by the Section 1 (*Atomic Collision Processes*).

The SPIG 2014 will be held from 26th to 29th August in Belgrade, Serbia. The details of the conference are available at www.spig2014.ipb.ac.rs. Unfortunately, due to the limited conference budget, the organizers cannot commit to any financial support.

We hope that you will be able to accept our invitation. Please let us know by the 4th of November and send us the title of your lecture.

We look forward to welcoming you to Belgrade in 2014.

Yours sincerely,

Mijatović Zoran

Marić Dragana A. Milosavljević

Zoran Mijatović
(Chairman of the
Scientific Committee)

Dragana Marić and **Aleksandar R. Milosavljević**
(Co-Chairs of the Local Organizing Committee)

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Mijatović Zoran Marić Dragana A. Milosavljević

Zoran Mijatović (Chairman of the Scientific Committee)

Dragana Marić and **Aleksandar R. Milosavljević** (Co-Chairs of the Local Organizing Committee)

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KINETIC ENERGY DISTRIBUTION OF ELECTRONS SCATTERED INSIDE A PLATINUM TUBE AT THE INCIDENT ENERGY OF 200 eV

A. R. Milosavljević [1,*], M. Lj. Ranković [1], J. B. Maljković [1], R. J. Bereczky [2],
B. P. Marinković [1] and K. Tőkési [2]

[1]Institute of Physics, University of Belgrade, Pregrevica 118, Belgrade, Serbia
[2] Institute for Nuclear Research, Hungarian Academy of Sciences, H-4001 Debrecen, Hungary, EU

Abstract. We have measured the kinetic energy distribution of electrons escaping a macroscopic platinum (Pt) tube (3.3 mm diameter and 40.8 mm length). The 200 eV incident electron beam of about 800 nA was directed into the capillary entrance at a large tilt angle of 5.5°, with respect to the capillary axis. The results show a dominant fraction of elastically scattered electrons, accompanied by inelastic losses.

1. INTRODUCTION

Insulating micro- and nano-capillaries made of different materials have been extensively used to investigate the so-called *guiding* phenomenon, which was first revealed with the pioneering work of Stolterfoht and coauthors in 2002 [1]. Briefly, the beam of charged particles, particularly highly charged ions (HCI), dinamically deposit charge on the inner capillary surface, thus providing a Coulomb field that deflects the particles and efficiently guides them towards the capillary exit. Large attention has been devoted to this phenomenon due to both an interesting physics and possible applications, such as the possibility to introduce a micro/nano HCI beam directly into a biological object [2]. The first results on electron guiding through insulating capillaries have been reported more recently [3,4], followed by a more detailed investigations [5,6]. A comprehensive review on the subject can be found in the recent paper by Lemell et al. [7].

In contrast to the HCI, the electron transmission through insulating capillaries appeared to be much more complex [5,6,7]. Particularly, electrons can be closely elastically scattered from the surface (not only deflected by deposited charge), inelastically scattered and can produce secondary electrons (which thus affect the Coulomb interaction). Moreover, it has been suggested that even metallic (conductive) capillaries could be used for the electron guiding [6].

In the present work, we investigate electron transmission through metallic macroscopic capillaries. Our aim is both to learn about fundamental properties of the electron guding by metallic capillaries, governed by electron-surface interaction, and to investigate the potential application of metallic high-aspect ratio capillaries as a robust, spatially well-determined, low-energy electron carier/source, which could be efficiently applied to study electron driven molecular processes under different environmental conditions. We started investigation with a large-diameter Pt tube, in order to compare the obtained results to the electron interaction with a plane Pt surface and theoretical simulations. In the present work, we have investigated transmission of 200 eV incident electrons through a single Pt macrocapillary (3.3 mm diameter and 40.8 mm length – the aspect ratio of about 12.4). The intensity of the outgoing electron current has been measured as a function of both the incident beam angle with respect to the capillary axis (tilt angle) and the kinetic energy of outgoing electrons.

2. EXPERIMENTAL SETUP

The experiment has been performed in the Laboratory for Atomic Collision Processes, at the Institute of Physics Belgrade (IPB) by using the electron spectrometer UGRA [8], which has been modified to perform the present experiment. The electron gun produces a well collimated electron beam, with a diameter and an angular divergence estimated to be approximately 1 mm and 1° at 200 eV of the incident energy, and with an energy spread of about 0.5 eV. The Pt tube has been fitted inside the entrance electron lens system (see Figure 1), in front of the electron gun, which can be rotated around the capillary entrance in the angular domain of about -15 to +15 degrees. The angle between the capillary axis and incident electron beam direction is denoted as the tilt angle.

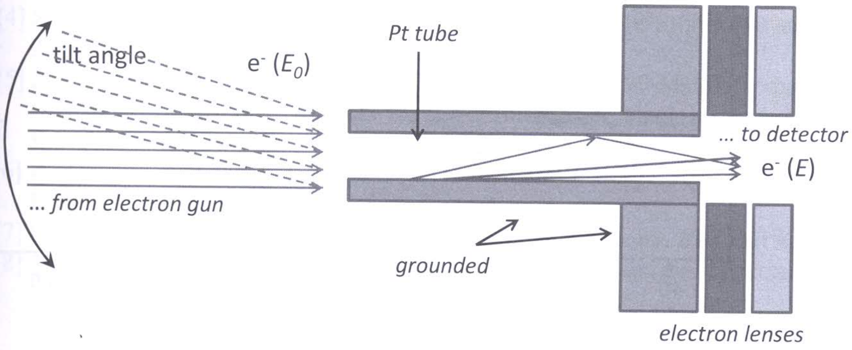

Figure 1. Schematic drawing of the experimental setup.

The electrons escaping the capillary were focused by an electrostatic lens (Figure 1) into a double cylindrical mirror energy analyzer (DCMA), followed by a single channel multiplier used as a detector. Since the entrance lens of the analyzer is fixed to have its axis parallel to the capillary axis, the observation angle is fixed at 0° and the acceptance angle also depends on the focal properties of the entrance lens. The kinetic energy distribution of the electrons escaping the capillary was measured by recording the electron current at the detector (count rates) as a function of the retarding potential at the entrance of the DCMA that worked in a constant pass-energy mode, thus providing a constant energy resolution over the whole scanned energy domain [8]. Still, it should be noted that the recorded kinetic energy distribution can be affected by the transmission of the entrance lens [8].

3. RESULTS

The preliminary obtained kinetic energy distribution of electrons escaping the Pt tube at the tilt angle of about 5.5° and for the incident electron energy of 200 eV is shown in Figure 2.

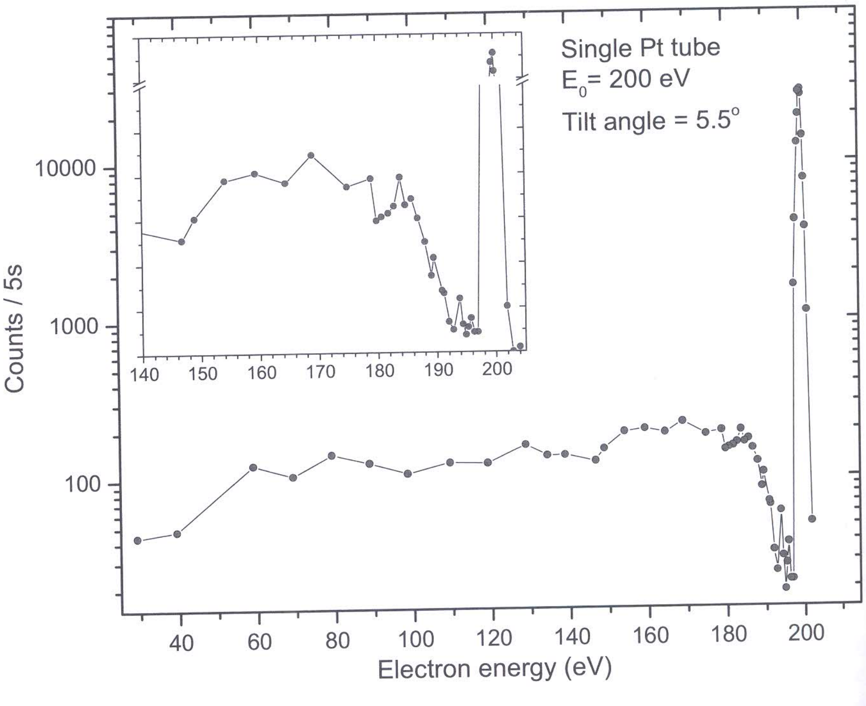

Figure 2. The kinetic energy distribution of electrons escaping the Pt tube at the tilt angle of 5.5° and the incident electron energy of 200 eV.

The aspect ratio of the Pt tube defines the tilt angle of 4.6° as a maximum angle to transmit the direct electron beam. Moreover, even at smaller tilt angles down to only a few degrees, the electron detection should not be possible due to the aspect ratio of the entrance lens stack and the DCMA (see Figure 1), which also depends on the electrostatic field. Therefore, the present results suggest that 200 eV electrons can be directed and transmitted along the metallic Pt tube. The dominant fraction of the transmitted electrons seems to suffer only elastic surface collisions. Inelastically scattered electrons are also detected and further work is in progress to compare the present results with the electron scattering from a plane Pt surface and calculations that include cylindrical geometry.

Acknowlendgements

The work was supported by the Ministry of education, science and technological development of Republic of Serbia under the grant OI 171020, by the Hungarian SRF OTKA No. NN 103279, and by the Bilateral Cooperation Program between the Hungarian and Serbian Academies. The work is also motivated by ESF/COST Action CM1301 "Chemistry for Electron-Induced Nanofabrication (CELINA).

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SPIG 2014 PROGRAM

Belgrade, Serbia, August 26 – 29, 2014

Tuesday 26th August 2014

Workshops

	DEA Workshop
08:30-09:00	Registration
09:00-09:10	Opening and Introduction Nigel Mason (Open University)
	Session 1, Hall A, *Chair: Nigel Mason*
09:10-09:30	*Electron attachment to molecules studied by electron-molecular crossed beam experiment* **Janina Kopyra,** Siedlce University, Siedlce, Poland
09:30-09:50	*Electron attachment to unstable molecules* **Tom Field,** Queen's University of Belfast, Belfast, UK
09:50-10:10	*Dissociative electron attachment studies with potential radiosensitizers* **Stephan Denifl,** University of Innsbruck, Institute of Ion Physics, Innsbruck, Austria
10:10-10:30	*(Time-dependent) Density Functional Theory for understanding dissociative chemistry of organometallic compounds* **Matija Zlatar,** Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia
10:30-11:00	***Coffee break***
	Session 2, Hall A, *Chair: Oddur Ingólfsson*
11:00-11:20	*Dissociation of polar molecules at very low energies* **Roman Čurík,** J. Heyrovský Institute of Physical Chemistry of the ASCR, Prague, Czech Republic
11:20-11:40	*Role of symmetry lowering in DEA* **Juraj Fedor,** Department of Chemistry, University of Fribourg, Fribourg, Switzerland
11:40-12:00	*Velocity slice imaging study on dissociative electron attachment* **Ewelina Szymanska,** Department of Physical Sciences, The Open University, Milton Keynes, UK
12:00-12:20	*Theoretical treatment of dissociative electron attachment* **Peter Papp,** Comenius University, Bratislava, Slovakia
12:20-13:50	***Lunch break (&registration)***

	XiBiGP Workshop	***NonEqProc Workshop***
13:50-14:00	Opening and Introduction Christophe Nicolas (SOLEIL synchrotron)	Opening and Introduction Zoran Lj. Petrovic (SASA)
	Session 1, Hall A *Chair: Christophe Nicolas*	***Session 1, Hall B*** *Chair: Saša Dujko*
14:00-14:30	*Study of single photon multiple ionization processes with a magnetic bottle spectrometer* **Pascal Lablanquie,** LCP-MR CNRS & Université Paris VI, Paris, France	*Non-equilibrium transport of charged particles in gaseous and disordered materials* **Ron White,** ARC Centre of Excellence for Antimatter-Matter Studies, James Cook University, Townsville, Australia
14:30-15:00	*Synchrotron radiation studies of biomolecules: photoabsorption, and core and valence photoionization* **Kevin Prince,** Sincrotrone Trieste, Trieste, Italy	*First principles calculation of the effect of Coulomb collisions on electron swarms* **Zoltan Donko,** Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary
15:00-15:30	*Electron-ion coincidence spectroscopy as a tool to study radiation-induced molecular dynamics* **Edwin Kukk,** Department of Physics and Astronomy, University of Turku, Turku, Finland	*Recent progress in the Newtonian three-body problem* **Veljko Dmitrašinović and Milovan Šuvakov,** Institute of Physics, Belgrade, Serbia

15:30-16:00	***Coffee break and discussion***	
	Session 2, Hall A *Chair: Lidija Andrić*	***Session 2, Hall B*** *Chair: Marija Radmilović-Rađenović*
16:00-16:30	*Biomolecular ionization and fragmentation dynamics studied with energetic photons from synchrotrons and free electron lasers* **Thomas Schlathölter,** University of Groningen, Groningen, Netherlands	*Emission spectroscopy of dense plasmas in liquids: a winding road from light to chemistry* **Thierry Belmonte,** *Institut Jean Lamour, Université de Lorraine, Nancy, France*
16:30-17:00	*Action spectroscopy of stored biomolecular ions in the soft X-ray range* **Alexandre Giuliani,** Synchrotron SOLEIL, France/**Aleksandar Milosavljević**, Institute of Physics, University of Belgrade, Belgrade, Serbia	*Picosecond-TALIF to probe atomic oxygen in the plume of an RF driven atmospheric pressure plasma jet in ambient air* **Jérôme Bredin,** The University of York, York, UK
17:00-17:30	*Proton transfer and non-local electronic relaxation in aqueous solutions revealed from core-level autoionization* **Bernd Winter,** BESSY, Germany	*Comparison of surface vacuum ultraviolet emissions with resonance level number densities in Argon and Argon containing plasmas* **Svetlana Radovanov,** Applied Materials/Varian Semiconductor, USA
17:30-18:00	***Coffee break***	
	Joint Session (XiBiGP & NonEqProc), Hall A *Chair: Bratislav Marinković*	
18:00-18:30	*Spectral analysis from physics for optimization of magnetic resonance spectroscopy in early tumor diagnostics* **Karen Belkić,** Karolinska Institute, Stockholm, Sweden	
18:30-19:00	*Measuring elementary plasma processes: Elastic scattering, vibrational and electronic excitation, dissociative attachment* **Michael Allan,** University of Fribourg, Switzerland	
19:00-19:30	*Future Studies on Electron Scattering; a Renaissance?* **Nigel Mason,** The Open University, Milton Keynes United Kingdom	
19:30-22:00	***Welcome party (Gallery of Science and Technology, SASA) –*** *concert “Ca va” (Prague)*	

Wednesday 27th August 2014

SPIG 2014 (day 1)

(***PL** – Plenary lecture: 35+10 min;* ***TL** – Topical lecture: 25+5 min;* ***PR** – Progres Report: 15+5 min*)

08:00-09:15	Registration	
09:15-09:45	**Opening, Chair: Zoran Mijatović**	
	***Plenary Session 1, Hall A**, Chair: Zoran Lj. Petrović*	
09:45-10:30	*Plasma Medicine: Fundamentals and Applications* **Alexander Fridman,** Drexel University, Philadelphia, USA	
10:30-11:00	***Coffee break***	
	***Plenary Session 2, Hall A**, Chair: Luka Popović*	
11:00-11:45	*What happens at the surface impact site of a slow highly charged ion?* **Friedrich Aumayr,** Vienna University of Technology (TU Wien), Vienna, Austria	
11:45-12:30	*Fifty Years of QUASARS: Physical Insights and Potential for Cosmology* **Jack Sulentic,** Instituto de Astrofísica de Andalucía – CSIC, Granada, Spain	
12:30-14:30	***Lunch break***	
	Parallel session A1, *Chair: Aleksandar Milosavljević*	***Parallel session B1,*** *Chair: Bratislav Obradović*
14:30-15:00	*Positron interactions with atoms and molecules* **Stephen Buckman,** The Australian National University, Canberra, Australia	*A CCP-plasma source operation in the high-VHF to UHF frequencies and scalability to large-area applications* **Albert R. Ellingboe,** Dublin City University, Dublin, Ireland
15:00-15:30	*Chirality reveals electronic/nuclear motion couplings* **Gustavo Garcia,** Synchrotron SOLEIL, France	*Application of low temperature plasmas for restoration/conservation of archaeological objects* **František Krčma,** Brno University of Technology, Brno, Czech Republic
15:30-15:50	*Stability of nucleosides in the gas phase under ionizing radiation* **Sylvain Maclot,** Université de Caen Basse-Normandie, Caen, France	*Treatment effects and stability of metal substrates treated by cold surface DBD plasma* **Vadym Prysiazhnyi,** Faculty of Engineering, UNESP, Guaratingueta, Brazil
15:50-16:30	***Coffee break***	
	Parallel session A2, *Chair: Dragana Marić*	***Parallel session B2,*** *Chair: Vladimir Srećković*
16:30-17:00	*Liquid-phase reactions induced by atmospheric pressure glow discharge with liquid electrode* **Fumiyoshi Tochikubo,** Tokyo Metropolitan University, Tokyo, Japan	*Anion chemistry in Titan* **Janko Zabka,** J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic
17:00-17:20	*Atmospheric Pressure Plasma Jet interactions with liquids* **Sylwia Ptasinska,** Notre Dame University, Notre Dame, USA	*Langmuir Waves in Interplanetary Plasma* **Sonja Vidojević,** IHIS – techno experts d.o.o, Belgrade, Serbia
17:20-17:40	*Low temperature plasma for medical applications* **Ita Junkar,** Jožef Stefan Institute, Ljubljana, Slovenia	*Studying the complex absorption profiles of Si IV in 21 HiBALQSO spectra* **Dimitrios Stathopoulos,** National and Kapodistrian University of Athens, Greece

17:40-18:00	*Monte Carlo modeling of positron transport in experimental devices and applications* **Srđan Marjanović,** Institute of Physics, University of Belgrade, Belgrade, Serbia	*Dynamic Effects in Excited Atomic Systems* **Andrei Klyucharev,** Saint-Petersburg University, St.-Petersburg, Russia
18:00-19:30	***Poster session (1) -*** *Gallery of Science and Technology, SASA* *Posters: 1.20 – 1.33; 2.1 – 2.19; 3.1 – 3.24*	

Thursday 28th August 2014		
SPIG 2014 (day 2)		
(***PL*** *– Plenary lecture: 35+10 min;* ***TL*** *– Topical lecture: 25+5 min;* ***PR*** *– Progres Report: 15+5 min*)		
	Plenary Session 3, Hall A*, Chair: Nikola Konjević*	
09:00-09:45	*The role of high-energy ion-atom/molecule collisions in radiotherapy* **Dževad Belkić,** Department of Oncology and Pathology, Nobel Medical Institute, Karolinska Institute, Stockholm, Sweden	
09:45-10:30	*Study of a High-Performance Plasma in the Large Helical Device* **Akio Komori,** National Institute for Fusion Science, Gifu, Japan	
10:30-11:00	***Coffee break***	
	Plenary Session 4, Hall A*, Chair: Bratislav Marinković*	
11:00-11:45	*The two sides of the electron in FEBID: Fragmentation of molecules and molecular synthesis* **Petra Swiderek ,** University of Bremen, Bremen, Germany	
11:45-12:30	*Recent Results for Electron Scattering from Atoms and Molecules* **Michael Brunger,** Flinders University, Adelaide, Australia	
12:30-14:30	***Lunch break***	
	Parallel session A3, *Chair: Stephen Buckman*	***Parallel session B3,*** *Chair: Nevena Puač*
14:30-15:00	*Latest developments in low energy electron-molecule scattering: the R-matrix approach* **Jimena Gorfinkiel,** Open University, Milton Keynes, UK	*Deposition of innovative coatings by DBD at atmospheric-pressure* **David Duday,** CRP - Gabriel Lippmann, Belvaux, Luxembourg
15:00-15:30	*Low-energy electron-induced bond cleavage studied in DNA at a single-molecule level* **Ilko Bald,** Universität Potsdam, Potsdam-Golm, Germany	*The afterglow of a surface-wave microwave discharge as a tool for surface process studies* **Kinga Kutasi,** Hungarian academy of sciences, Budapest, Hungary
(A) 15:30-15:50 (B) 15:30-16:00	*Electron attachment to c-C_4F_8O: dynamics and implications for plasmas* **Radmila Janečkova,** Department of Chemistry, University of Fribourg, Fribourg, Switzerland	*Plasma synthesis and processing of carbon nanowalls and submicron metallic particles* **Gheorghe Dinescu,** National Institute for Laser, Plasma and Radiation Physics, Magurele, Romania
15:50-16:30	***Coffee break***	

	Parallel session A4, *Chair: Petra Swiderek*	***Parallel session B4,*** *Chair: Saša Dujko*
(A) 16:30-16:50 (B) 16:30-17:00	*Molecular clusters: radiation induced processes and methods to control neutral beams* **Marcin Dampc,** The Open University, Milton Keynes, UK	*The IST-LISBON database on LXcat* **Luís Lemos Alves,** Instituto de Plasmas e Fusão Nuclear, Lisboa, Portugal
(A) 16:50-17:10 (B) 17:00-17:30	*Low energy electron interaction with typical focused electron beam induced deposition precursor* **Rachel Thorman,** University of Iceland, Reykjavik, Iceland	*Optical diagnostics of laboratory analogue of TLE discharges (Transient Luminous Events)* **Milan Šimek,** Academy of Sciences of the Czech Republic, Prague, Czech Republic
(A) 17:10-17:40 (B) 17:30-18:00	**COST CELINA lecture** *Event by event modelling procedure to simulate electron beam induced deposition* **Gustavo Garcia,** *CSIC, Madrid, Spain*	*canceled* Atsushi M. Ito, National Institute for Fusion Science, Gifu, Japan
17:40-18:00 (A)	*COST CELINA WG1 Meeting*	
18:00-19:30	***Poster session (2) -*** *Gallery of Science and Technology, SASA* *Posters: 1.1 – 1.19, 1.34 and 1.35; 3.25 – 3.52; 4.1 – 4.9*	
19:30-20:00	***Concert (Gallery of Science and Technology, SASA): quartet "Full Harmony"***	

Friday 29th August 2014	
SPIG 2014 (day 3)	
(***PL*** *– Plenary lecture: 35+10 min;* ***TL*** *– Topical lecture: 25+5 min;* ***PR*** *– Progres Report: 15+5 min*)	
	Plenary Session 5, Hall A*, Chair: Gordana Malović*
09:00-09:45	*Recent developments in positronium physics* **David Cassidy,** University College London, London, UK
09:45-10:30	*Laser ablation in liquids during nanoparticle production* **Alessandro De Giacomo,** University of Bari, Dipartimento di Chimica, Bari, Italy
10:30-11:00	***Coffee break***
	Plenary Session 6, Hall A*, Chair: Milorad Kuraica*
11:00-11:45	*Modelling of physical and chemical processes in cold atmospheric-pressure plasma jets* **George Naidis,** Institute for High Temperatures, RA S, Moscow, Russia
11:45-12:30	*Attosecond VUV Coherent Control of Molecular Dynamics and Perspectives For Using ELI-ALPS User Facility* **Predrag Ranitović,** Lawrence Berkeley National Laboratory, Berkeley, California, USA
12:30-14:30	***Lunch break / SPIG Committee meeting at 13h***

	Parallel session A5, *Chair: Goran Poparić*	***Parallel session B5,*** *Chair: Milivoje Ivković*
14:30-14:50	*Electron transfer upon potassium collisions with biomolecules* **Filipe Ferreira da Silva,** *Universidade Nova de Lisboa, Portugal*	*Electrical breakdowns in air: new experiments and statistical and numerical models* **Aleksandar Jovanović,** University of Niš, Serbia
14:50-15:10	*Absolute differential cross sections for elastic electron scattering from small biomolecules* **Jelena Maljković ,** Institute of Physics, University of Belgrade, Belgrade, Serbia	*Spectroscopic study of plasma during electrolytic oxidation of magnesium-aluminium alloys* **Jovica Jovović,** Faculty of Physics, University of Belgrade, Belgrade, Serbia
15:10-15:30	*Electron – Indium atom scattering and analysis of electron and optical spectra* **Maja Rabasović,** Institute of Physics, University of Belgrade, Belgrade, Serbia	*Measurements and models of transient and stationary regimes of glow discharge in argon* **Marjan Stankov,** University of Niš, Niš, Serbia
15:30-15:50	*Single electron capture in fast ion-atom collisions* **Nenad Milojević,** University of Niš, Serbia	*Diagnostics of Laser induced plasma by optical emission spectroscopy* **Marko Cvejić,** Institute of Physics, University of Belgrade, Belgrade, Serbia
15:50-16:30	***Coffee break***	
	Parallel session A6, *Chair: Zoltan Donkó*	***Parallel session B6,*** *Chair: Nenad Simonović*
(A) 16:30-16:50 (B) 16:30-17:00	*Electron heating dynamics in multi-frequency capacitive RF discharges* **Aranka Derzsi,** Hungarian academy of sciences, Budapest, Hungary	*Electron excitation and autoinization cross sections for elements of chemically peculiar (CP) stars: Study of bismuth* **Branko Predojević,** University of Banja Luka, Banja Luka, Repubika Srpska, B&H
(A) 16:50-17:10 (B) 17:00-17:20	*Simulation and modeling of Resistive Plate Chambers* **Danko Bošnjaković,** Institute of Physics, University of Belgrade, Belgrade, Serbia	*Wake effect in graphene due to moving charged particles* **Ivan Radović,** VINCA Institute of Nuclear Sciences, Belgrade, Serbia
(A) 17:10-17:30 (B) 17:20-17:40	*The non-symmetric ion-atom absorption processes in the helium rich white dwarf atmospheres in UV and EUV region* **Vladimir Srećković,** Institute of Physics, University of Belgrade, Belgrade, Serbia	*Interaction of charged particles with capillaries* **Károly Tőkési,** Institute for Nuclear Research, Hungarian Academy of Sciences, Debrecen, Hungary
	Free time	
20:00	***Gathering and transport to Danube quay***	
20:30 -	***Conference dinner and Closing***	

Saturday 30th August 2014	
10:00-17:00	***Excursions (optional, info at registration desk)***
17:00	***Departure***

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SPIG 2014

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August 26-29, 2014, Belgrade, Serbia

CONTRIBUTED PAPERS
&
ABSTRACTS OF INVITED LECTURES, TOPICAL INVITED LECTURES, PROGRESS REPORTS AND WORKSHOP LECTURES

Editors:
Dragana Marić
Aleksandar R. Milosavljević
Zoran Mijatović

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2nd Annual Meeting, 6th - 9th May 2015, Hotel SOREA Regia, Bratislava, Slovakia

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2nd Annual Meeting of COST Action CM 1301, CELINA

Chemistry for ELectron-Induced NAnofabrication

6th – 9th May, 2015, Bratislava, Slovakia

Book of Abstracts

Local Organizer:	**Peter Papp**	**(Comenius University in Bratislava, Slovakia)**
Action Chair:	**Petra Swiderek**	**(University of Bremen, Germany)**

Electron impact dissociative ionization of tetraethyl orthosilicate

Jelena Maljković[1], Peter Papp[2], Michal Lacko[2], Michal Stano[2], Aleksandar Milosavljević[1], Stefan Matejcik[2]

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(2) Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská dolina, 84248 Bratislava, Slovakia

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We have investigated dissociative electron ionization of tetraethyl orthosilicate, TEOS ($Si(OC_2H_5)_4$), in gas phase, interesting as a possible Focused Electron Beam Induced Dissociation (FEBID) precursor. Measurements were performed at Comenius University on the crossed beams apparatus [1] and the cluster apparatus [2]. Both are equipped with trochoidal electron monohromator, which produces well collimated electron beam crossed perpendicularly with target. Positive ions formed with electron molecular interactions are extracted by a small electric field and recorded by quadrupole mass analyser. We have measured the possible pattern of fragmentation for TEOS molecule and compared with the NIST mass spectrum. Beside parent $M=(Si(OC_2H_5)_4)^+$ at m/z 208 many other positive ions were recorded in the mass spectrum, with many SiO_x^+ fragments (x= 2, 3 and 4) and their hydrogenated alternatives between m/z 60 and 100. Only the loss of 1 or 3 CH_3 or C_2H_5 was typical for TEOS, contrary to the loss of 1 or all 4 OC_2H_5 ligands. Alternative fragmentation paths were the loss of 2 CH_3 + CH_2CH_3; CH_3 + C_2H_5 + OC_2H_5; 2 C_2H_5 + OC_2H_5; CH_3 + 2 C_2H_5 + OC_2H_5. Beside that, measurements of threshold energies for all TEOS fragments have been done.

This work was supported by the Slovak Research and Development Agency under Contract No. APVV-0733-11; the Slovak grant agency VEGA V/0514/12; Ministry of Education and Science of Republic of Serbia (Project No. 171020). This work was conducted within the framework of the COST Action CM1301 (CELINA).

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	Wednesday 6th May, 2015	Thursday 7th May, 2015	Friday 8th May, 2015	Saturday 9th May, 2015	
09:00		**WG3 (30m)** **Stefan F. Rohrlack**	**WG2 (40m)** **Anjana Devi**		09:00
09:30	STSMs reports (20m)	**WG2 (30m)** **Mats Tilset**		**WG3 (30m)** **Willem van Dorp**	09:30
09:40			WG1 Petr Carsky		09:40
10:00		WG1 Rachel Thorman	WG1 Maciej Gutowski	WG1 Jelena Maljkovic	10:00
10:20		**Coffee**	**Coffee**	**Coffee**	10:20
10:40		WG1 Andrew Ellis	WG3 Hans Mulders	WG1 Ragesh Kumar	10:40
11:00		WG1 Juraj Fedor	WG1 Lionel Amiaud	WG1 André Beyer	11:00
11:20		WG3 Jelena Tamuliene	WG3 Francesc Salvat-Pujol	WG3 Sangeetha Hari	11:20
11:40		WG1 Jonas Warneke	WG3 Thomas Verduin	**Lunch** **&** **Departures**	11:40
12:00		**Lunch**	**Lunch**		12:00
13:30	**REGISTRATION**	**Posters** **&** **MC Meeting**	**COST CM1301** **WG** **Meetings**		13:30
15:40		**Coffee**			15:40
16:00		**WG3 (40m)** **Michael Huth**	**Conference** **Excursion**		16:00
16:40		**WG2 (30m)** **Heinrich Lang**			16:40
17:10		WG2 Iwona Szymanska			17:10
17:30		WG3 Marijke Scotuzzi			17:30
17:50	Opening	WG1 Alex Laikhtman			17:50
18:00	**WG1 (40m)** **Howard Fairbrother**		**Conference** **Dinner**		18:00
18:10		**Individual** **Dinner** **in the** **City**			18:10
18:40	**WG1 (30m)** **Stefan Matejcik**				18:40
19:10	**Welcome** **Reception**				19:10

Journal of Physics: Conference Series

Study of electron transmission through a metallic capillary

To cite this article: A R Milosavljevi *et al* 2015 *J. Phys.: Conf. Ser.* **635** 062011

Study of electron transmission through a metallic capillary

A. R. Milosavljević[1], M. Lj. Ranković[1*], D. Borka[2], J. B. Maljković[1], R. J. Bereczky[3], B. P. Marinković[1] and K. Tőkési[3]

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Synopsis In this work we study the transmission of charged particles through a single cylindrically shaped metallic capillary of microscopic dimensions with a large aspect ratio. We used electrons as projectiles. Our results suggest the existence of guiding of the electron beam by a metallic capillary.

In this work we investigate the guiding of electrons through straight and narrow metallic capillaries. The investigation of guiding of charged particles by metal capillaries is strongly motivated by the possibility of producing cheap alternatives to complex electron-optical tools.

We have performed both the measurements and the classical calculations of electrons guiding [1, 2, 3]. Since electrons cannot change their charge state, it is experimentally impossible to make a clear distinction between transmission of the primary and secondary electrons which correspond to elastic scattering. But using the classical simulation, we can identify and follow up all electron trajectories. We performed Monte Carlo simulation assuming that after each inelastic collision a secondary electron is generated with kinetic energy directly estimated from the energy transfer [2, 3]. The created secondary electron is treated as a primary electron and the trace of its path is followed in the successive simulation procedure.

Our experimental setup consisted of an electron gun, a straight cylindrical platinum capillary, an energy analyzer and a channeltron as a detector. Pressure inside the vacuum chamber was $7\text{x}10^{-7}$ mbar. An inner radius of the capillary was 3.3 mm, with 40.8 mm in length. Estimated electron beam width at the entrance of the capillary was 0.9 mm with 0.3° angle divergence. The initial electron energy was 200 eV. We found that a dominant fraction of electrons escaping from the capillary have energies smaller than the incident electron energy. Figure 1. shows the energy spectrum of electrons transmitted through a cylindrical platinum capillary.

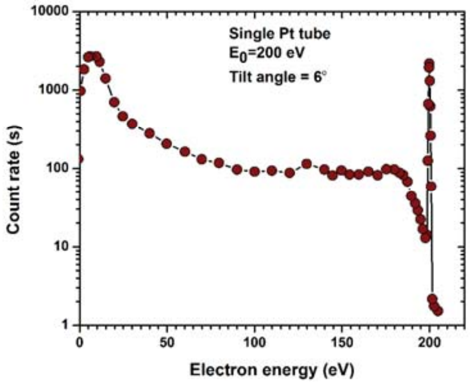

Figure 1. - Energy spectrum of electrons transmitted through platinum capillary [4].

This work was supported by the Ministry of education, science and technological development of Republic of Serbia under the Grants OI 171020 and III 45005, by the Hungarian SRF OTKA No. NN 103279, and by the Bilateral Cooperation Program between the Hungarian and Serbian Academies. This work was conducted within the framework of the COST Action CM1301 (CELINA).

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[3] B.S. Dassanayake, R.J. Bereczky, S. Das, A. Ayyad, K. Tőkési, J.A. Tanis *2011 Phys. Rev. A* **83** 012707.
[4] Milosavljevic et al, NIMB 2015

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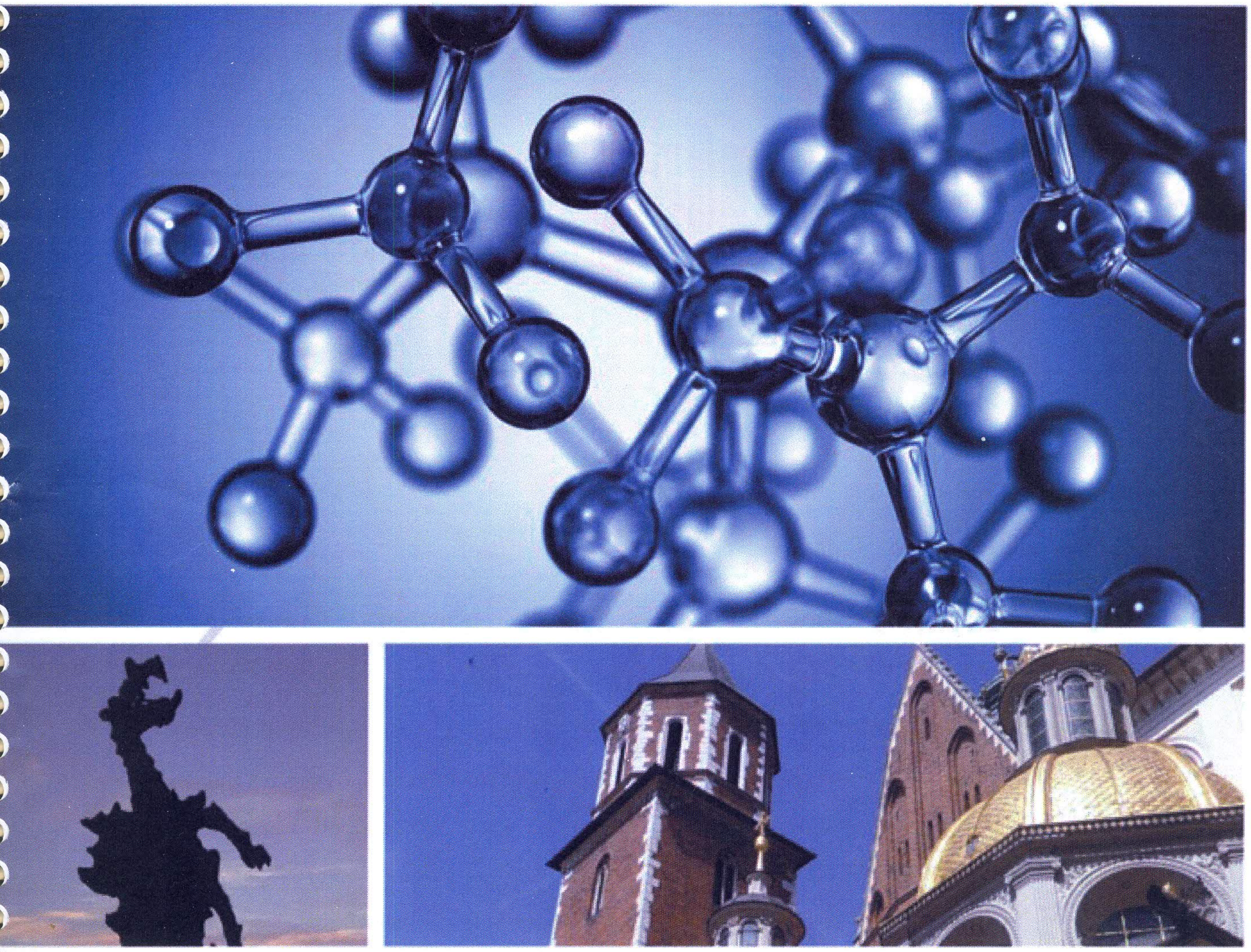
15:20 - 15:40	***Jelena Maljkovic*** *(University of Belgrade, Serbia)* Dissociative electron attachment to benzene chromium tricarbonyl
15:40 - 16:00	***Anita Ribar*** *(Leopold-Franzens-Universität Innsbruck, Austria)* Low-Energy Electron Interaction with Tungsten Hexacarbonyl Clusters
16:00 - 16:20	**Coffee break**
16:20 - 19:00	Poster Session
17:00 - 19:00	MC meeting
19:00 -	Individual dinner in the city

Thursday, 19th of May	
Chairman: Oddur Ingolfsson	
9:00 - 9:40	***Simon Elliott*** *(University College Cork, Ireland)* Introduction to Atomic Layer Deposition and the COST Action HERALD
9:40 - 10:10	***Armin Gölzhäuser*** *(Universität Bielefeld, Germany)* Nanopore Fabrication and Characterization by Helium Ion Microscopy
10:10 - 10:40	***Charlene Lobo*** *(University of Technology Sydney, Australia)* Electron beam processes for surface functionalization and directed nanostructure assembly semiconductors
10:40 - 11:00	**Coffee break**
Chairman: Petra Swiderek	
11:00 - 11:30	***Hartmut Hotop*** *(University of Kaiserslautern, Germany)* Michael Allan - electron impact spectroscopy at its best
11:30 - 12:00	***Ilya Fabrikant*** *(University of Nebraska, USA)* Resonances and Threshold Effects in Electron Collisions with Molecules and Clusters
12:00 - 12:30	***Roman Curik*** *(Academy of Sciences of the Czech Republic, Czech Republic)* Negative ion resonances of polyatomic molecules: are they relevant for search of FEBID precursors?
12:30 - 13:00	***Juraj Fedor*** *(Academy of Sciences of the Czech Republic, Czech Republic)* Cluster-beam experiments and the insight they bring into FEBID
13:00 - 15:00	Lunch
15:00 - 18:30	Conference excursion: Krakow Old Town Walk
18:30 -	Conference dinner

CELINA

cost
EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY



The 3rd CELINA Meeting

Kraków, May 18-20, 2016

Subject **COST CELINA 2016_Invitation**
From CELINA 2016 <celina2016@uph.edu.pl>
To <jelenam@ipb.ac.rs>
Date 2016-03-31 18:34
Priority Normal

Dear Dr Jelena Maljkovic,

On behalf of the organizers I would like to invite you to give a 20 min talk (15 + 5 min) on your recent work at the annual meeting of the COST Action CM1301 on Chemistry for Electron-Induced Nanofabrication (CELINA). The meeting will be held in Krakow, Poland the 18th to 20th of May 2016.

http://www.celina.uni-bremen.de/celina/celina2016

Please notify me at the earliest opportunity if you can accept this invitation.

Yours sincerely,
Janina Kopyra

DISSOCIATIVE ELECTRON ATTACHMENT TO BENZENE CHROMIUM TRICARBONYL

Jelena Maljković [1*], Paulina Maciejewska [2] and Janina Kopyra [2]

[1] *Laboratory for Atomic Collision Processes, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[2] *Faculty of Sciences, Siedlce University, 3 Maja 54, 08-110 Siedlce, Poland*

Abstract. We have investigated dissociative electron attachment to benzene chromium tricarbonyl, M = $C_r(C_6H_6)CO_3$. This molecule was in our interest because it is a possible Focused Electron Beam Induced Dissociation (FEBID) precursor. Measurements were done utilizing an experimental setup settled in Siedlce, Poland. The obtained mass spectra were recorded for the energies from 0 eV to 14 eV, with 2 eV step. The compound showed a very rich fragmentation pattern.

1. INTRODUCTION

In the present work a dissociative electron attachment (DEA) to benzene chromium tricarbonyl has been investigated. In DEA processes electron is captured by molecule forming a temporary negative ion, which can decompose into negative fragment and one or more neutral counterparts. This molecule has been in our interest because it is potential Focused Electron Beam Induced Deposition (FEBID) precursor. FEBID is a direct-writing technique in which the metallic deposit is deposited onto a substrate with nanometer resolution. In this technique a highly focused, high-energy electron beam impinges on a substrate and due to collisions produces lower energy back-scattered electrons and secondary electrons. It is nowadays very well known that these low energy electrons (LEEs) contribute to the processes resulting in the formation of the deposits. However, in the case when LEEs lead to partial fragmentation of the target molecules this results in the formation of deposit with limited purity and resolution.

The benzene chromium tricarbonyl molecule belongs to organometallic compounds. It has piano stool geometry with planar arrangement of aryl group and three carbonyl groups which act as “legs” (Figure 1). This molecule has been investigated previously. Rees and Copens [1] have been studied the crystal structure of this molecule at 78 K, both by X-ray and neutron difraction. The electronic structure of transition metal in benzene chromium tricarbonyl has been investigated by using SCF MO calculations [2]. Uemura and coauthors [3] have investigated direct regioselective lithiation of chromium benzenetricarbonyl.

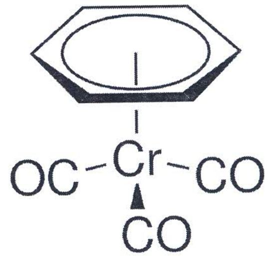


Figure 1. Structure of benzene chromium tricarbonyl molecule.

2. EXPERIMENT

The experiments were performed by means of crossed beam apparatus settled at Siedlce University, Poland. Description of the experimental set-up has been given elsewhere [4]. Briefly, it consists of a trochoidal electron monochromator (TEM), a quadrupole mass analyzer (QMA) and a secondary electron multiplier, all enclosed into vacuum chamber. Incident electron beam, with energy resolution of FWHM= 150-200meV and electron current I≈10nA, orthogonally intersects with molecular beam resulting in the formation of fragment anions. Molecular beam emanates from the oven which was heated by two halogen bulbs. These lamps prevent condensation of the target molecules at the lenses and also provide sufficient vapour pressure of the target molecules and also and provide stabile experimental conditions. Working temperature was around 95 °C. Negative ions are extracted directly from the collision region by a small electric field, towards a QMA and detected by single pulse counting techniques. The calibration of the energy scale was achieved by measuring SF_6 signal, with intense resonance near 0 eV. Base pressure was in the range of $\sim 10^{-8}$ mbar while the working pressure around 3×10^{-5} mbar.

3. RESULTS

Preliminary results of dissociative electron attachment to benzene chromium tricarbonyl are shown. Resonant features of anion yields indicate that underlying processes are DEA, as the only effective below ionization energy, IE ≈7eV [5]. Mass spectra has been obtained in the incident electron energy range from 0 eV up to 14 eV. Molecule showed rich anion formation: $(M - CO)^- = 186$ a.m.u., $(M - (CO)_2)^- = 158$ a.m.u, $(M - (CO)_3)^- = 130$ a.m.u, $(M - C_6H_6)^- = 136$ a.m.u, $Cr^- = 52$ a.m.u., $Cr(CO)^- = 80$ a.m.u, $(Cr(CO)_2)^- = 108$ a.m.u. and $Cr(CO)^-$ = 80 a.m.u. The most intense reaction channel is the loss of one carbonyl group, which is also shown by other authors [6] in DEA process to $W(CO)_6$. Reaction channel associated with loss of all three CO groups, Figure 2, has a threshold around 3eV. Three resonances are present in the anion yield curve. We can speak here about metastabile decays, also shown in [6]. Sequential process, where $(M - CO)^-$ decays to $(M - (CO)_2)^-$ and $(M - (CO)_2)^-$ decays to $(M - (CO)_3)^-$ can occur in this presently studied compound.

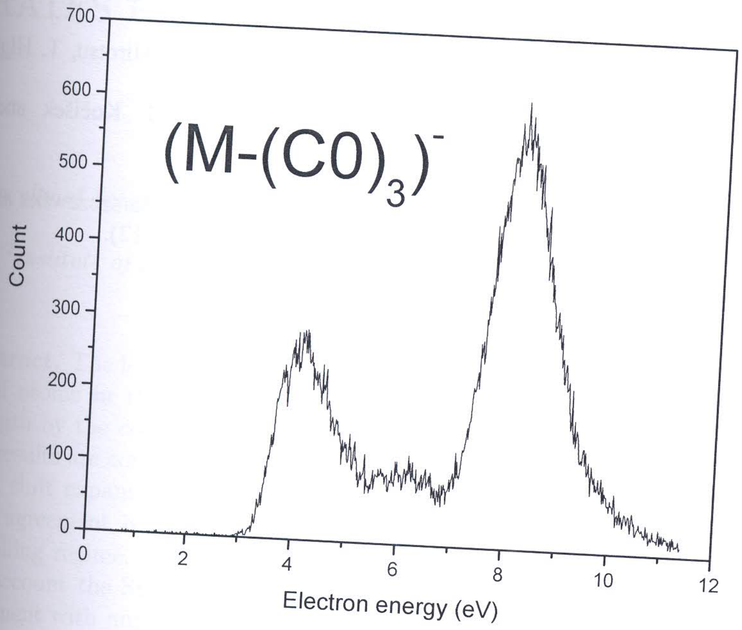


Figure 2. Anion yield of $(M - (CO)_3)^-$ formed by electron impact.

4. CONCLUSION

DEA processes have been investigated on benzene chromium tricarbonyl, a potential FEBID precursor. The obtained action tandem mass spectra have showed rich anion formation. The release of one, two and three CO groups has been noticed that is a consequence of a prompt decomposition of the temporary negative ion. In addition, a sequential processes can contribute to the overall intensity of the above mentioned fragment anions.

Acknowledgements

This work was supported by the Polish Ministry of Science and Higher Education (Project No. 277/S/11), Ministry of Education and Science of Republic of Serbia (Project No. 171020). This work was conducted within the framework of the COST Action CM1301 (CELINA).

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SPIG 2016

28th Summer School and
International Symposium on
the Physics of Ionized Gases
Aug. 29 - Sep. 2, 2016, Belgrade, Serbia

CONTRIBUTED PAPERS
&
ABSTRACTS OF INVITED LECTURES, TOPICAL INVITED LECTURES, PROGRESS REPORTS AND WORKSHOP LECTURES

Editors:
Dragana Marić, Aleksandar Milosavljević,
Bratislav Obradović and Goran Poparić

University of Belgrade,
Faculty of Physics

Serbian Academy
of Sciences and Arts

CEPAS 2017

7th Conference on Elementary Processes in Atomic Systems

3rd – 6th September 2017

Průhonice, Czech Republic

Electron transmission through steel capillary

B.P. Marinković[1], M.Lj. Ranković[1], J.B. Maljković[1], A.R. Milosavljević[2], D. Borka[3], C. Lemell[4], K. Tőkesi[5]

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[2] *PLÉIADES beamline, Synchrotron SOLEIL, L'orme des Merisiers, Saint-Aubin - BP48, 91192 GIF-sur-YVETTE CEDEX, France*

[3] *Atomic Physics Laboratory, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia*

[4] *Institute for Theoretical Physics, Vienna University of Technology, Vienna, Austria*

[5] *Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary and ELI-ALPS, ELI-HU Non-profit Kft., Szeged, Hungary*

The transmission of low-energy electrons through platinum [1, 2] and steel capillaries have been investigated both experimentally and theoretically. The length of the present steel capillary was $L =$ 19.50 mm while the inner diameter was $d = 0.90$ mm. Kinetic energy distribution of electrons transmitted through steel capillary was recorded at two tilt angles (the angle between the incident electron beam and the capillary axis) of 2.64° and 4.0°, respectively. The experimental results were obtained by an electron spectrometer which consists of an electron gun, a double cylindrical mirror energy analyzer (DCMA) and a channeltron detector.

Electron transmission is modelled by a classical trajectory Monte Carlo simulation taking both elastic and inelastic scattering events of primary electrons colliding with the inner wall of the capillary and transport of secondary electrons into account.

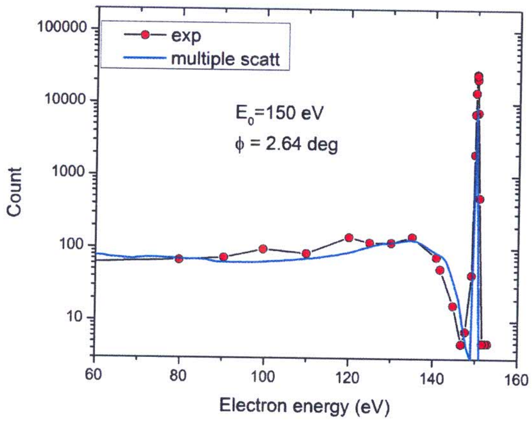


Figure 1: Energy spectra of electrons transmitted through a steel capillary.

Figure 1 shows energy spectra of 150 eV electrons passing through the steel capillary at 2.64° tilt angle. We found excellent agreement between our simulated electron-energy spectra with experimental data.

[1] A.R. Milosavljević *et al.*. Nucl. Instr. Meth. Phys. Res. B **354** (2015) 86.
[2] D. Borka *et al.*, Nucl. Instr. Meth. Phys. Res. B, in press (2017), http://dx.doi.org/10.1016/j.nimb.2017.02.024

CELINA 2017 Porto Portugal

	Wednesday 13/09/2017	Thursday 14/09/2017	Friday 15/09/2017	Saturday 16/09/2017
08:45 - 09:00		Opening		
09:00 - 09:20		Petra Swiderek	Juraj Fedor	Mostafa M. Shawrav
09:20 - 09:30		José Maria de Teresa		
09:30 - 09:50			Matija Zlatar	Anpan Han
09:50 - 10:00		Armin Gölzhäuser (Ion beam)		
10:00 - 10:20			Juraj Orzsagh	Markus Rohdenburg (STSM)
10:20 - 10:40		Teodor Gotszalk (STSM)	Anita Ribar (STSM)	Katja Höflich
10:40 - 11:10		Coffee	Coffee	Coffee
11:10 - 11:30		Iwona Szymanska	Gregor Hlawacek (Ion beam)	Janina Kopyra
11:30 - 11:40				Sylwia Ptasinska
11:40 - 11:50		Ivo Utke	Lisa McElwee-White	
11:50 - 12:00				Gian Carlo Gazzadi (STSM)
12:00 - 12:10		Katarzyna Madajska (STSM)		
12:10 - 12:20			Discussion on future activites (WG meetings)	Sascha Koch
12:20 - 12:30		Lionel Amiaud		
12:30 - 12:50				Concluding remarks
12:50 - 14:00		Lunch	Lunch	Lunch
14:00 - 14:30	Registration	Sven Barth	Walking tour	Departure
14:30 - 15:00		Oddur Ingolfsson		
15:00 - 15:30		Michael Huth		
15:30 - 15:50		Ragesh Kumar (STSM)		
15:50 - 19:00		Poster session MC meeting		
19:00 - open end			Conference dinner	

🟩	CELINA overview and synthetic perspectives
⬛	Novel developments in FEBID and beyond
🟦	Carboxylate precursors
🟧	Bimetallic precursors
🟨	Neutral excitation and dissociation
🟥	Process gases for deposit purification and lithography
🟩	Improved control over electron-driven processing
🟦	General 0

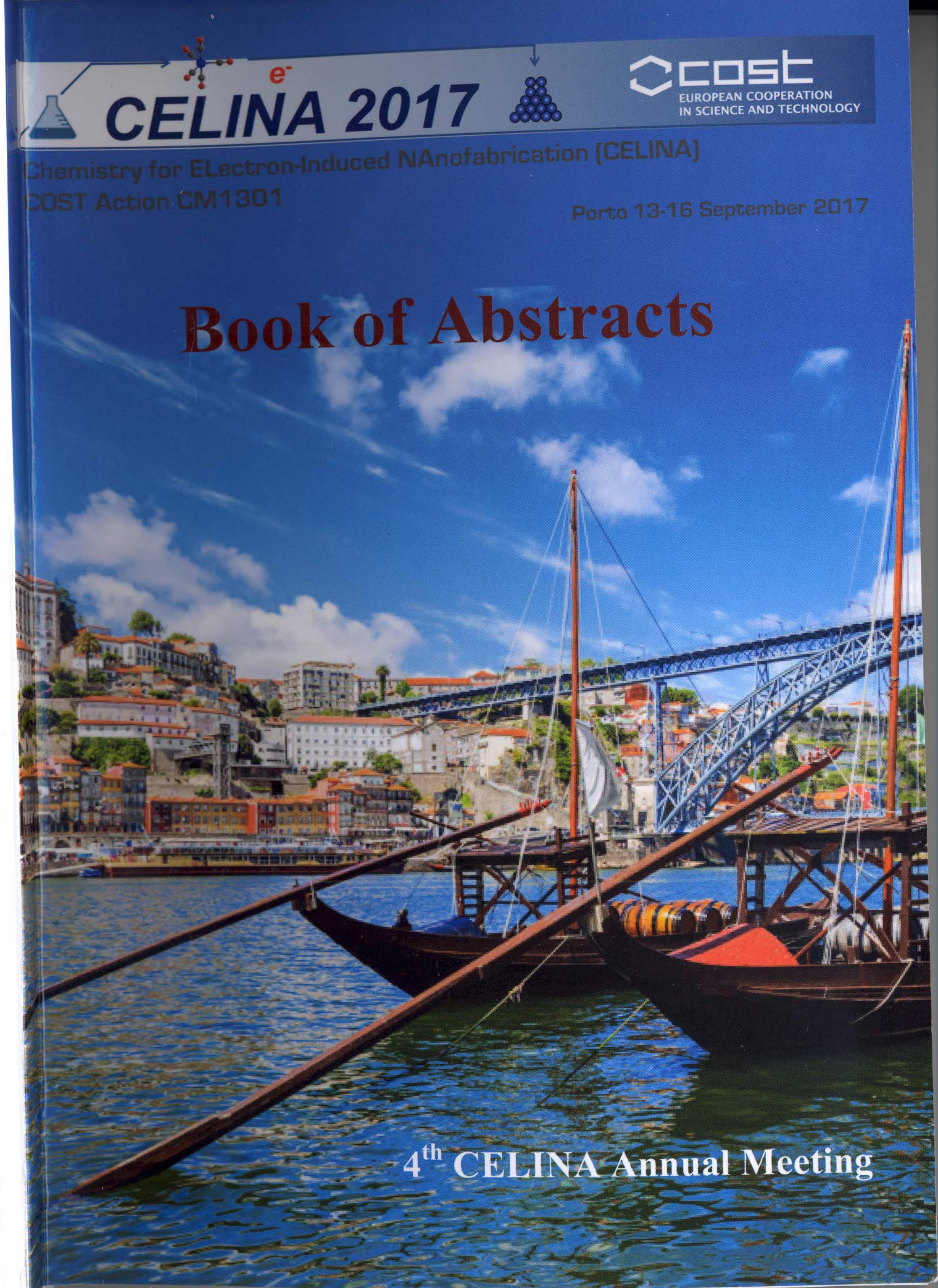
CELINA 2017

EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

Chemistry for ELectron-Induced NAnofabrication (CELINA)
COST Action CM1301

Porto 13-16 September 2017

Book of Abstracts



4th CELINA Annual Meeting

P-11: Dissociative electron attachment to cyclopentadienylmanganese(I) tricarbonyl

Jelena Maljković[1]*, Sylwia Mazuryk[2], and Janina Kopyra[2]

[1] Laboratory for Atomic Collision Processes, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia
[2] Faculty of Sciences, Siedlce University, 3 Maja 54, 08-110 Siedlce, Poland

In the present work a dissociative electron attachment (DEA) to cyclopentadienylmanganese(I) tricarbonyl, $(C_5H_5)Mn(CO)_3$, has been investigated. Molecule can be considered as potential FEBID precursor. This samle has extremely high sublimation rate and adsorb on filament of ion gauge, so measurements were hard to perform. Measurements were done utilizing an experimental setup [1] settled in Siedlce, Poland. Briefly, it consists of trochoidal electron monochromator (TEM), quadrupole mass analyzer (QMA) and secondary electron multiplier, all enclosed into vacuum chamber. Incident electron beam, with energy resolution of FWHM ≈ 160meV, orthogonally crossed with molecular beam resulting in the formation of fragment anions. The obtained mass spectra were recorded for the energies from 0 eV to 8 eV, with 2 eV step. The compound showed weak features, at energy near 0 eV, that are due to the loss of one or two carbonyl groups: $(M - CO)^-$ = 176 a.m.u., $(M - (CO)_2)^-$ = 148 a.m.u. Temperature was around 45°C and the pressure around $4.4\times10\text{-}^{7}$ mbars.

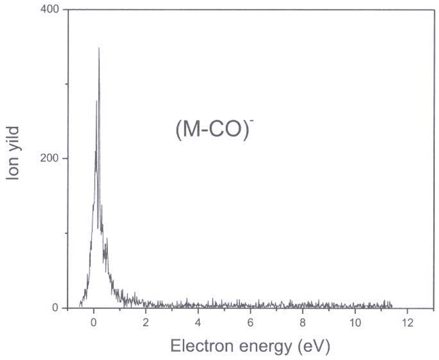


Fig.1. Ion yield of $(M-(CO))^-$, produced from electron impact on gaseous cyclopentadienylmanganese(I) tricarbonyl.

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MPS '18
Budapest

INTERNATIONAL CONFERENCE ON MANY PARTICLE SPECTROSCOPY OF ATOMS, MOLECULES, CLUSTERS AND SURFACES

BUDAPEST, HUNGARY
21-24 AUGUST 2018

PROGRAMME AND BOOK OF ABSTRACTS

International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces

Budapest, Hungary

21-24 August 2018

MPS '18

Budapest

Programme
and
Book of Abstracts

Local Organizing Committee

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Web address: mpsbudapest2018.com **E-mail**: mpsbudapest2018@gmail.com

Organized by

EKHO' 94 Ltd., Debrecen

Venue

Danubius Hotel Flamenco, Budapest, 3-7 Tas vezér str., 1113

Conference Issue

Papers submitted to the conference will be published following the conference in a Topical Issue (Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces) of EPJD: Atomic, Molecular, Optical and Plasma Physics.
Guest Editors: K. Tőkési, B. Paripás, G. Pszota, and A V Solov'yov

Programme and Book of Abstracts

This book contains the programme of the International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces held from 21-24 August 2018 in Budapest. Hungary and

the camera-ready copies of the abstracts as sent by the authors. In few cases only minor corrections were made.
Editors: K. Tőkési, B. Paripás, G. Pszota

Printed by: Rexpo Ltd.
ISBN 978-615-00-2859-0

Preface

Welcome to the International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces, MPS-2018, organized in Budapest, Hungary, from 21 to 24 August 2018. The objective of MPS-2018 is to assess the state of the art in the current understanding of a variety of basic phenomena in the charged particle dynamics in atoms, molecules, clusters and at surfaces such as a) collision induced physical, chemical and biological reactions, b) ultrafast dynamics, c) charge-exchange processes, d) collective as well as single-particle excitation and ionization, e) electron-electron correlation effects in atoms and in solids, f) excitation and single and multiple ionization of various targets, g) energy loss, scattering and channeling of primary particles, and h) electron and photon emission processes.

MPS is a biannual meeting. The aim is to promote the growth and exchange of scientific information on these areas of atomic and molecular and surface physics. The most recent meetings have been held in Moscow (Russia, 2016) Metz (France, 2014), Berlin (Germany, 2012), Sendai (Japan, 2010), Paris (France, 2008), Rome (Italy, 2006).

Hungary is a landlocked country in the Carpathian Basin in Central Europe, bordered by Austria, Slovakia, Ukraine, Romania, Serbia, Croatia and Slovenia. Its capital is Budapest. Hungary has been a member state of the European Union since 1 May 2004.

The conference is held at the Danubius Hotel Flamenco (Address: 3-7 Tas vezér str., 1113 Budapest), the most modern conference centre in Budapest.

Hotel Flamenco offers something rare – accommodation close to the centre of Budapest yet surrounded by beautiful parkland. This four-star hotel near the so-called "Bottomless Lake" in Budapest's 11th district has its own garage and rooftop car park, although it's also easily accessible by public transport with metro, bus and tram stops a short walk away. Hotel Flamenco is also an ideal venue for events. Its conference rooms come in various sizes, making it equally suitable for hosting smaller conferences and major events for several hundred people.

We hope that all participants will have a lively and successful meeting while enjoying the attractive surroundings in this beautiful region of Hungary. We hope, furthermore, we may offer exciting scientific programs and last but not least famous Hungarian dishes and wines. Organizers have been doing their best to guarantee pleasant experiences for everyone.

On behalf of the local organizing committee,

Károly Tőkési

Chair of MPS-2018

International Advisory Board

Scientific Program

August 2018, Tuesday

16:00 – 20:00 Registration
18:00 – 19:30 Cheese and wine reception

22 August 2018, Wednesday

Femto-, attosecond physics and imaging (Chair: Edwin Kukk)

8:40 – 9:00	***Opening***	Károly Tőkési, Norbert Kroó
9:00 – 9:30	***Fernando Martin*** Universidad Autónoma de Madrid, Spain	***Attosecond coupled electron and nuclear dynamics in molecules***
9:30 – 10:00	***Nora Berrah*** University of Connecticut, Storrs, USA	***C60 femtosecond dynamics induced by the LCLS X-ray FEL***
10:00 – 10:30	**Florian Trinter** DESY, Hamburg, Germany	***Imaging the correlated two-electron wave function of a hydrogen molecule***

Coffee Break (10:30 – 11:00)

Photoionization I. (Chair: Emma Sokell)

11:00 – 11:30	***Liang-You Peng*** Peking University, Beijing China	***Few-photon double ionization of Helium***
11:30 – 11:50	***Maria-Novella Piancastelli*** Sorbonne Université, Paris, France	***Photoexcitation and photoionization dynamics of isolated atoms and molecules in the tender x-ray domain***
11:50 – 12:10	***Stephan Fritzsche*** Universität Jena, Germany	***Excitation and ionization of atoms by twisted light***
12:10 – 12:30	***Francis Penent*** Sorbonne Université, Paris, France	***Multiple photoionization of alkali atoms***

Lunch (12:30 – 14:00)

Laser field I. (Chair: Nora Berrah)

14:00 – 14:30	***Elena V. Gryzlova*** Lomonosov Moscow State University, Russia	***Ionic autoionizing states studied with free-electron lasers***
14:30 – 15:00	***Diego G. Arbó*** IAFE (UBA-CONICET), Buenos Aires, Argentina	***Retrieving intracycle interference in angle-resolved laser assisted XUV atomic ionization***
15:00 – 15:20	***Philipp V. Demekhin*** Universität Kassel, Germany	***Correlative two-electron dynamics in helium driven by intense laser pulses***
15:20 – 15:40	***Barna Imre*** Wigner Research Centre for Physics, Budapest, Hungary	***Electron scattering and conduction in doped semiconductors in simultaneous strong infrared radiation field***

Coffee Break (15:40 – 16:10)

Laser field II. (Chair: Alisher Kadyrov)

16:10 – 16:40	***Akiyoshi Hishikawa*** Nagoya University, Japan	***Photoelectron transversal momentum distribution from D2 in circularly polarized intense laser fields***
16:40 – 17:10	***Nicolas Camus*** MPIK, Heidelberg, Germany	***Experimental studies of Wigner's tunnelling time***

17:10 – 18:30 Poster session (P1 - P54)

23 August 2018, Thursday

Photoionization II. (Chair: Shaofeng Zhang)

9:00 – 9:30	***Nicolas Sisourat*** Sorbonne Université, Paris, France	***Interatomic Coulombic Decay in triatomic and more complex systems***
9:30 – 9:50	***Eliezer Kolodney*** Technion - Israel Institute of Technology, Haifa Israel	***Postcollision (delayed) fission and multifragmentation in fullerene-surface impact: experiment and simulation***
9:50 – 10:10	***Yuki Orimo*** The University of Tokyo, Japan	***Ab initio simulations of photoelectron energy spectra from multielectron systems subject to intense laser fields***
10:10 – 10:30	***Stepan Balybin*** Lomonosov Moscow State University, Russia	***Enhancement of ionization of atoms in bright squeezed vacuum light***

Coffee Break (10:30 – 11:00)

Interactions with molecules I. (Chair: Lorenzo Avaldi)

11:00 – 11:30	***Da Bo*** National Institute for Materials Science, Tsukuba, Japan	***Virtual Substrate Method for Nanomaterials Characterization***
11:30 – 11:50	***Victor Despre*** Universitat Heidelberg, Germany	***Charge migration in propiolic acid and its dephasing by the coupling to the nuclear motion***
11:50 – 12:10	***Moustafa Zmerli*** Sorbonne Université, Paris(05), France	***Charge transfer and nuclear dynamics after methyl iodide core ionization following single photon absorption***
12:10 – 12:30	***Raimund Feifel*** University of Gothenburg, Sweden	***Ultrafast molecular three-electron collective Auger decay***

Lunch (12:30 – 14:00)

Interactions with molecules II. (Chair: Sebastian Otranto)

14:00 – 14:30	***Miriam Weller*** Goethe-Universität Frankfurt, Germany	***Time-resolved Studies of Molecular Systems Using Synchrotron Radiation***
14:30 – 15:00	***Kilian Fehre*** Goethe-Universität Frankfurt, Germany	***Strong Field Ionization of Chiral Molecules***
15:00 – 15:20	***Mohammad F. Gharaibeh*** Qatar University, Doha, Qatar	***K-shell photoionization of molecular oxygen-ions***
15:20 – 15:40	***Nikolay Shvetsov*** Leibniz Universität Hannover, Germany	***Semiclassical two-step model and strong-field ionization of hydrogen molecule***

Coffee Break (15:40 – 16:10)

More complex systems (Chair: Piero Decleva)

16:10 – 16:40	***Péter Dombi*** Wigner Research Centre for Physics, Budapest, Hungary	***Photoelectron spectroscopy for ultrasensitive measurement of plasmon fields***
16:40 – 17:00	***Hicham Agueny*** University of Bergen, Norway	***Electron dynamics in single-cycle THz pulses***

17:00 – 18:30 Poster session (P55 – P108)

19:30 – Conference dinner

24 August 2018, Friday

Electron collisions (Chair: Alexander Dorn)

9:00 – 9:30	***Jelena Maljković*** Institute of Physics Belgrade, Serbia	***Elastic electron scattering by triethyl phosphate molecule – experimental and theoretical study***
9:30 – 10:00	***Zehra N. Ozer*** Afyon Kocatepe University, Afyon, Turkey	***Experimental and theoretical investigation of triple differential cross sections of CO_2 molecule at intermediate electron energy***
10:00 – 10:30	***Matthieu Genevriez*** Universit e Catholique de Louvain, Belgium	***Absolute cross section for electron-impact ionization of He(1s2s ^3S)***

Coffee Break (10:30 – 11:00)

Collision with molecular systems (Chair: Stephan Fritzsche)

11:00 – 11:30	***Noboru Watanabe*** Tohoku University, Sendai, Japan	***Stereodynamics in electron-impact ionization of molecules studied by molecular-frame electron energy loss spectroscopy***
11:30 – 11:50	***Vishant Kumar*** Normandie Université, Caen, France	***Investigating the fragmentation dynamics and geometry of CO molecular clusters***
11:50 – 12:10	***Zoltán Jurek*** Center for Free-Electron Laser Science, Hamburg, Germany	***Chemical dynamics in Argon clusters induced by intense x-rays***
12:10 – 12:30	***Isabella Floss*** Vienna University of Technology, Austria	***Multi-scale simulation of high harmonic generation in condensed matter***

Lunch (12:30 – 14:00)

Heavy particle collisions (Chairs: Nicolas Sisourat/ Nikolay Shvetsov-Shilovskiy)

14:00 – 14:30	***Ilkhom Abdurakhmanov*** Curtin University, Perth, Australia	***Calculating fully differential cross section for ionization of H and He by heavy projectiles***
14:30 – 14:50	***Richard A. Wilhelm*** Vienna University of Technology, Austria	***Ultrafast neutralization dynamics of highly charged ions upon impact on atomically thin solid targets"***
14:50 – 15:10	***Luca Repetto*** Università di Genova, Italy	***Ion induced self-organization of form birefringent Cr-Si subwavelength optical gratings***
15:10 – 15:30	***Alisher Kadyrov*** Curtin University, Perth, Australia	***Quantum suppression of antihydrogen formation in positronium-antiproton collisions***
15:30 – 15:50	***Örs Asztalos*** Budapest University of Technology and Economics, Hungary	***Application of Collisional Radiative models in Beam Emission Spectroscopy modeling for fusion plasma density diagnostics***
15:50 – 16:10	***Sebastian Otranto*** Instituto de Física del Sur Bahía Blanca, Argentina	**Ion impact ionization of H_2O at intermediate energies: the role of multiple electron removal**

16:10 – Final remarks

16:30 – End of Meeting

Invited lecturers

Ilkhom Abdurakhmanov
Calculating fully differential ionization cross section of H and He upon heavy projectile impact
Department of Physics, Astronomy and Medical Radiation Sciences, Curtin University, GPO Box U1987, Perth 6845, Australia

Diego Arbó
Retrieving intracycle interference in angle-resolved laser assisted XUV atomic ionization
Institute for Astronomy and Space Physics - IAFE, Buenos Aires, Argentina

Nora Berrah
X-ray induced time-resolved dynamics in Fullerenes
University of Connecticut Department of Physics, USA

Nicolas Camus
Experimental studies of Wigner's tunneling time
Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Bo Da
Virtual Substrate Method for Nanomaterials Characterization
Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan

Péter Dombi
Photoelectron spectroscopy for ultrasensitive measurement of plasmon fields
Wigner Research Centre for Physics, Budapest

Kilian Fehre
Strong Field Ionization of Chiral Molecules
Institut für Kernphysik, Johann Wolfgang Goethe Universität, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

Matthieu Génévriez
Absolute cross section for electron-impact ionization of He(1s2s 3S)
Laboratory for Physical Chemistry, ETH Zürich, Switzerland.

Elena Gryzlova
Ionic autoionizing states studied with free-electron lasers
Lomonosov Moscow State University, Skobeltsyn Institute of Nuclear Physics, Moscow, Russia

Akiyoshi Hishikawa
Manipulating atoms and molecules by intense laser fields
Department of Chemistry, Graduate School of Science, Nagoya University, Nagoya, Japan

Jelena Maljković
Elastic electron scattering by triethyl phosphate molecule – experimental and theoretical study
Institute of Physics Belgrade, Serbia

Fernando Martin
Attosecond coupled electron and nuclear dynamics in molecules
Departamento de Química, Módulo13, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Zehra Nur Özer
Experimental and theoretical investigation of triple differential cross sections of CO2 molecule at intermediate electron energy
Afyon Kocatepe University, Physics Department, Turkey

Laing-You Peng
Few-Photon Double Ionization of Helium.
School of Physics, Peking University, 100871, Beijing, China

Nicolas Sisourat
Interatomic Coulombic Decay in triatomic and more complex systems
Sorbonne Universités, UPMC Univ Paris 06, CNRS, Laboratoire de Chimie Physique Matière et Rayonnement, F-75005, Paris, France

Florian Trinter
Imaging the correlated two-electron wave function of a hydrogen molecule
Deutsches Elektronen-Synchrotron (DESY), FS-PE, Notkestrasse 85, 22607 Hamburg, Germany and Fritz-Haber-Institut der Max-Planck-Gesellschaft, Molecular Physics, Faradayweg 4, 14195 Berlin, Germany

Noboru Watanabe
Stereodynamics in electron-impact ionization of molecules studied by molecular-frame electron energy loss spectroscopy
Institute of Multidisciplinary Research for Advanced Materials Tohoku University, Sendai, Japan

Miriam Weller
Timeresolved Studies of Molecular Systems Using Synchrotron Radiation
Institut für Kernphysik, Goethe-University Frankfurt am Main, Germany

Elastic electron scattering by triethyl phosphate molecule – experimental and theoretical study

J. Vuković[1], *B. P. Marinković*[2], *B. Predojević*[1], *K. Tökési*[3,4], *J. Maljković*[2]

[1]*Faculty of Natural Sciences, University of Banja Luka, Republic of Srpska, Bosnia and Herzegovina*
[2]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[3]*Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary*
[4]*ELI-ALPS, ELI-HU Non-profit Kft., Szeged, Hungary*
Corresponding author: jelena.maljkovic@ipb.ac.rs

Electron elastic differential cross sections (DCS) of triethyl phosphate molecule $(C_2H_5)_3PO_4$ have been investigated both experimentally and theoretically. Beside its role as a polymer resin modifier or a common intermediate in the manufacture of pesticides [1], triethyl phosphate molecule can serve as a model for radiation damage of the phosphate group as a part of DNA backbone (Fig.1).

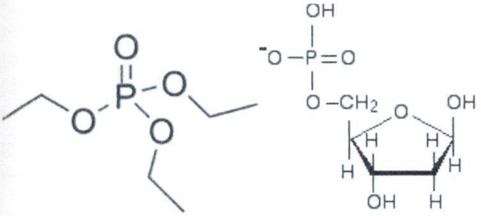

Figure 1. The skeletal formula of (*a*) triethyl phosphate molecule and (*b*) a phosphate group attached to the sugar molecule in place of the -OH group on the 5' carbon atom in DNA backbone.

The home-made experimental setup is based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron [2], while construction of a gas line used for relative fow technique, design and programming of digital acquisition system are detailed in [3]. DCS data as function of scattering angle, DCS (θ), is obtained by measuring the signal and background for each angle point. For the relative flow measurements argon gas was taken as a reference gas and the absolute cross sections have been used from the recent measurements in our group [4].

The partial expansion method was used to describe the differential and total cross sections for electron elastic scattering. The method of calculations can be found in reference [5].

Measurements have been performed at several electron impact energies, i.e. 50, 100, 150 200 and 250 eV and in the angular range from 25° to 125°. In Fig.2 measured and calculated DCS at 100 eV are shown. Both sets of data are arbitrary normalized at the same point at 40° scattering angle.

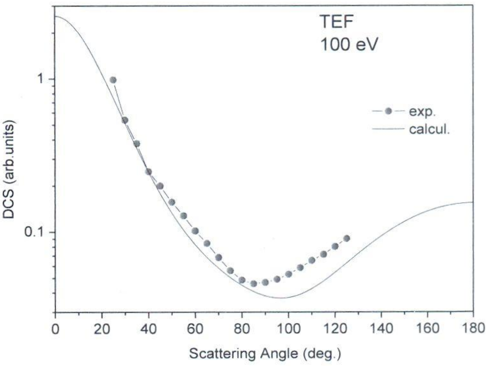

Figure 2. The experimental and calculated differential cross sections for electron elastic scattering by triethyl phosphate molecule at 100 eV impact energy. Both curves are normalized at scattering angle of 40 degrees.

The comparison in shape between experimental and calculated gives a good agreement. Still, we need to match the absolute scales and to estimate the uncertainities.

References

[1] D. Betteridge, M. Thompson, A.D. Baker, and N.R. Kemp, *Analytical Chem.*, (1972) 44, 2005.

[2] A.R. Milosavljević, S. Madžunkov, D. Šević, I. Čadež, B.P. Marinković, *J. Phys. B* (2006) **39**, 609.

[3] J.B. Maljković, A.R. Milosavljević, F. Blanco, D. Šević, G. García, B.P. Marinković, *Phys. Rev. A* (2009) **79**, 052706.

[4] Miloš Lj. Ranković, Jelena B. Maljković, Károly Tökési, and Bratislav P. Marinković, *Nucl. Instrum. Meth. B* **(2018) 72**, 30.

[5] F. Salvat, R. Mayol, *Comput. Phys. Commun.* (1993) **74**, 358

Absolute cross section for electron-impact ionization of He(1s2s ^{3}S)

M. Génévriez[*,†], **J. J. Jureta**[*], **P. Defrance**[*], **X. Urbain**[*]

[*] Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, Belgium
[†] Laboratory of Physical Chemistry, ETH Zurich, Zurich, Switzerland
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Electron-impact ionization of ground state helium is a benchmark process which, as such, has been extensively studied. Good agreement is now reached between the results of state-of-the-art theoretical and experimental investigations. The case of electron-impact ionization of the metastable, 1s2s ^{3}S state of helium is far from being as satisfactory. For example, despite sustained theoretical effort within the past decades, the only measurement of the absolute total ionization cross section which spans a significant energy range [4] lies more than 60% higher than the results of all recent, state-of-the-art calculations (see, *e.g.*, [3, 5]). This difference is not acceptable due to the importance of metastable helium in a wide variety of physical environments and processes, from Bose-Einstein condensates to diagnosis of thermonuclear fusion plasmas.

We have measured the absolute cross sections for electron-impact single and double ionization of He(1s2s ^{3}S) and for double ionization of He$^-$ [1], using the animated-crossed-beam technique of Defrance *et al.* [2]. A source of fast metastable helium atoms was purpose-built for this study and overcomes the lack of state selectivity existing in the earlier experiment. It is based on the photodetachment of fast (keV) He$^-$ ions by a CO$_2$ laser, which ensures that atoms are produced in the 1s2s ^{3}S state only. A relatively high beam brightness can be reached due to the large detachment efficiency, and purity is better than 5% with contamination limited to He(1s^2 ^{1}S) only.

The present results for single ionization of He(1s2s ^{3}S) lie significantly lower than the previous experiment, and are in fact in the region reached by recent, *ab initio* calculations [1]. They are in excellent agreement with the multicore calculation of Fursa and Bray [3], as shown in Fig. 1, over the whole energy range covered. Frozen-core calculations fail to match the present results at higher energies, hinting at significant contributions from inner-shell ionization and indirect mechanisms such as excitation to doubly excited states and autoionization.

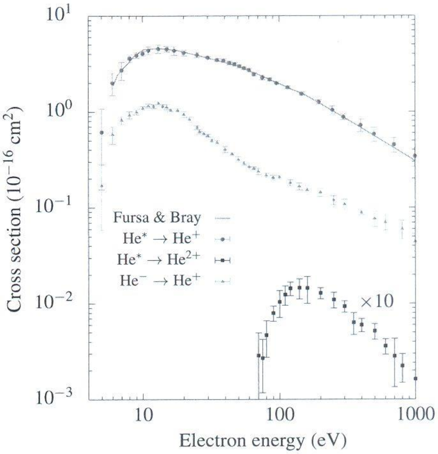

Figure 1. Cross sections for electron-impact single and double ionization of He(1s2s ^{3}S) and double ionization of He$^-$.

Results for the double ionization of metastable helium and He$^-$ are the first data reported in the literature for these processes. The cross section for double ionization of He(1s2s ^{3}S) has roughly the same magnitude as that for ground state helium, suggesting that ionization of the second (1s) electron is the limiting factor. The cross section for double ionization of He$^-$ is much larger than typical values, as expected for such a weakly bound system (77 meV), and does not match for universal shape of Rost and Pattard [6].

References

[1] M. Génévriez *et al.* 2017 *Phys. Rev. A* 96 010701(R)

[2] P. Defrance *et al.* 1981 *J. Phys. B* **14** 103

[3] D. V. Fursa and I. Bray 2003 *J. Phys. B* **36** 1663

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[5] Y. Ralchenko *et al.* 2008 *At. Data Nucl. Data Tables* **94** 603

[6] J. M. Rost and T. Pattard 1999 *J. Phys. B* **94** 603

August 22, 2018 Wednesday		**August 23, 2018 Thursday**		**August 24, 2018 Friday**	
Femto-, attosecond physics (Chair: Edwin Kukk)		Photoionization II. (Chair: Shaofeng Zhang)		Electron collisions (Chair: Alexander Dorn)	
8:40 – 9:00	*Opening* Norbert Kroó	9:00 – 9:30	*Nicolas Sisourat*	9:00 – 9:30	*Jelena Maljković*
9:00 – 9:30	*Fernando Martin*	9:30 – 9:50	*Eliezer Kolodney*	9:30 – 10:00	*Zehra N. Ozer*
9:30 – 10:00	*Nora Berrah*	9:50 – 10:10	*Yuki Orimo*	10:00 – 10:30	*Matthieu Genevriez*
10:00 – 10:30	*Florian Trinter*	10:10 – 10:30	*Stepan Balybin*		
10:30 – 11:00	**Coffee Break**	10:30 – 11:00	**Coffee Break**	10:30 – 11:00	**Coffee Break**
Photoionization I. (Chair: Emma Sokell)		Interactions with molecules I. (Chair: Lorenzo Avaldi)		Coll. with molecular syst. (Chair: Stephan Fritzsche)	
11:00 – 11:30	*Liang-You Peng*	11:00 – 11:30	*Da Bo*	11:00 – 11:30	*Noboru Watanabe*
11:30 – 11:50	*Maria-Novella Piancastelli*	11:30 – 11:50	*Victor Despre*	11:30 – 11:50	*Vishant Kumar*
11:50 – 12:10	*Stephan Fritzsche*	11:50 – 12:10	*Moustafa Zmerli*	11:50 – 12:10	*Zoltán Jurek*
12:10 – 12:30	*Francis Penent*	12:10 – 12:30	*Raimund Feifel*	12:10 – 12:30	*Isabella Floss*
12:30 – 14:00	**Lunch**	12:30 – 14:00	**Lunch**	12:30 – 14:00	**Lunch**
Laser field I. (Chair: Nora Berrah)		Interactions with molecules II. (Chair: Sebastian Otranto)		Heavy particle collisions (Chairs: Nicolas Sisourat/ Nikolay Shvetsov-Shilovski)	
14:00 – 14:30	*Elena V. Gryzlova*	14:00 – 14:30	*Miriam Weller*	14:00 – 14:30	*Ilkhom Abdurakhmanov*
14:30 – 15:00	*Diego G. Arbó*	14:30 – 15:00	*Kilian Fehre*	14:30 – 14:50	*Richard A. Wilhelm*
15:00 – 15:20	*Ph. V. Demekhin*	15:00 – 15:20	*Moh. F. Gharaibeh*	14:50 – 15:10	*Luca Repetto*
15:20 – 15:40	*Imre Barna*	15:20 – 15:40	*Nikolay Shvetsov-Shilovski*	15:10 – 15:30	*Alisher Kadyrov*
15:40 – 16:10	**Coffee Break**	15:40 – 16:10	**Coffee Break**	15:30 – 15:50 15:50 – 16:10	*Örs Asztalos* *Sebastian Otranto*
Laser field II. (Chair: Alisher Kadyrov)		More complex systems (Chair: Piero Decleva)		16:10 – 16:30	Final remarks
16:10 – 16:40	*Akiyoshi Hishikawa*	16:10 – 16:40	*Péter Dombi*	16:30	**End of the conference**
16:40 – 17:10	*Nicolas Camus*	16:40 – 17:00	*Hicham Agueny*		
17:10 – 18:30	**Poster session**	17:00 – 18:30	**Poster session**		
		19:30	**Conference dinner**		

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БЕОГРАД, СТУДЕНТСКИ ТРГ 12-16
П. ФАХ 44

ПОТВРДА

Овим се потврђује да је **др ЈЕЛЕНА МАЉКОВИЋ**, научни сарадник Института за физику руководила израдом мастер рада ЈЕЛЕНЕ ВУКОВИЋ под називом "АПСОЛУТНИ ПРЕСЕЦИ ЗА ЕЛЕАСТИЧНО РАСЕЈАЊЕ ЕЛЕКТРОНА НА МОЛЕКУЛУ ТРИЕТИЛ-ФОСФАТА", који је одбрањен на Физичком факултету Универзитета у Београду 24. septembra 2018. године.

Др Јелена Маљковић је за ментора мастер рада ЈЕЛЕНЕ ВУКОВИЋ именована на седници Наставно-научног већа Физичког факултета одржаној 18. oktobra 2017. године године.

Београд, 19.4.2022.

ДЕКАН ФИЗИЧКОГ ФАКУЛТЕТА

Проф. др Иван Белча

MPS '18
Budapest

The International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces MPS-2018 (21-24 August, 2018)

Date: Debrecen, 25. June 2018.

Dear Prof. Jelena Maljkovic!

As the chairman of the Local Organizing Committee of MPS'18 (The International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces), it is my pleasure to invite you to participate in the MPS'18 to be held in Budapest, Hungary from 21-24 August 2018.

Your contributed paper entitled *"Elastic electron scattering by triethyl phosphate molecule – experimental and theoretical study"* has been selected and accepted for invited talk presentation at the conference. MPS is a biannual meeting, which deals with physical and chemical phenomena induced by the interaction of charged particles (singly up to highly charged ions, atoms and clusters, electrons) and photons with atoms, molecules, clusters and surface and the bulk of solids and also liquids. The aim is to promote the growth and exchange of scientific information on these areas of atomic and molecular and surface physics.
Please note, however, that this invitation does not imply an obligation for financial support from the conference organizers.

The MPS-2018 organizers encourage you to apply for the visa (if needed) as early as possible. You may find more details concerning to visa issues on our official webpage: http://mpsbudapest2018.com

We are looking forward to welcoming you in Budapest!

Yours sincerely,

Prof. Dr. Károly Tőkési
Chairman
Conference Organizing Committee, MPS'18

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13. 04. 2022 год.
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П. ФАХ 44

ПОТВРДА

Овим се потврђује да је др Јелена Маљковић, научни сарадник Института за физику у Београду, ментор докторских студија Јелени Вукаловић, студенту треће године докторских студија на научној области Физика атома и молекула.

Београд, 12.04.2022.

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Проф. др Иван Белча

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FLORENCE, ITALY

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WELCOME

We are pleased to welcoming to the 13th European Conference on Atoms Molecules and Photons (ECAMP13) in Florence!

The triennial ECAMP conference series, launched in 1981, is the major conference of the Atomic, Molecular and Optical Physics Division (AMOPD) of the European Physical Society (EPS).

The Scientific Programme covers the most recent developments in the broader field of AMO physics.

We extend our sincere appreciation and gratitude to the Chairs and all Speakers whose contributions help to make this event possible.

We are very much looking forward to this outstanding event and its unique approach to exchanging knowledge.

The Local Organizing Committee

GENERAL INFORMATION

Organizing Committee

EPS AMOPD
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Organizing Secretariat

Viale Matteotti, 7 - 50121 Florence, Italy
Tel. ++39 055 50351 - Fax ++39 055 5001912
ecamp2019@oic.it - www.ecamp13.org

The Organizing Secretariat desk is open for registration and information according to the following time schedule:

Sunday, April 7	16.00-18.00
Monday, April 8	08.00-20.00
Tuesday, April 9	08.30-19.00
Wednesday, April 10	08.30-13.00
Thursday, April 11	08.30-19.00
Friday, April 12	08.30-17.30

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Delegates	600,00 € (491,80 € + VAT)
Students*	320,00 € (262,30 € + VAT)

*Copy of valid Student Card must be handed at the Registration Desk

Registration is mandatory for all oral and posters presenters.

Welcome Reception & Social Dinner for Accompanying Person

The price is 70,00 € (VAT included) and includes:
- Welcome reception on April 8 at the Congress Venue
- Social dinner on April 10 2019 at Palazzo Borghese

POSTER SESSION 3

P3.32 Symmetry breaking atomic ionization by coherent circularly polarized bichromatic radiation
E.V. Gryzlova[1], A.N. Grum-Grzhimailo[1], M.M. Popova[1], E.I. Staroselskaya[1], N. Douguet[2], K. Bartschat[2] ([1]Russia, [2]USA)

P3.33 Inspecting the hydrogen migration in water using asymmetric fs laser
E. Kechaoglou, S. Kaziannis, C. Kosmidis (Greece)

P3.34 Coherent blue light generated by four-wave mixing: interference effect and autler-townes splitting
M.P. Moreno, A.A.C. de Almeida, S.S. Vianna (Brazil)

P3.35 Coherent population oscillations–based light storage
P. Neveu, C. Banerjee, F. Bretenaker, E. Brion, F. Goldfarb (France)

P3.36 Phase sensitive amplification enabled by coherent population trapping
P. Neveu[1], C. Banerjee[1], J. Lugani[1,2], F. Bretenaker[1], E. Brion[1], F. Goldfarb[1] ([1]France, [2]United Kingdom)

P3.37 Elastic electron scattering from methane molecule in the energy range from 50-300eV
J.B. Maljković[1], J. Vuković[2], K. Tökési[3], B. Predojević[2], B.P. Marinković[1] ([1]Serbia, [2]Bosnia andHerzegovina, [3]Hungary)

P3.38 Calculation of elastic resonant electron scattering on one-electron Ions
K.N. Lyashchenko[1], D.M. Vasileva[1], O.Yu. Andreev[1], A.B. Voitki[2] ([1]Russia, [2]Germany)

P3.39 Laser-assisted (e,2e) ionization in a quasi-Sturmian-Floquet approach
S.A. Zaytsev[1], L.U. Ancarani[2], K.A. Kouzakov[1] ([1]Russia, [2]France)

Highly charged ions

P3.40 Towards background free studies of capture reactions in a heavyion storage ring
L. Varga[1], K. Blaum[1], T. Davinson[2], J. Glorius[1], B. Jurado[3], C. Langer[1], C. Lederer Woods[2], Yu.A. Litvinov[1], R. Reifarth[1], Z. Slavkovská[1], T. Stöhlker[1], P.J. Woods[1], Y.M. Xing[1] ([1]Germany, [2]United Kingdom, [3]France)

P3.41 Evidence of trielectronic recombination for Ar Ions in an EBIT
D.S. La Mantia[1,2], W. Biela[1], J.A. Tanis[2], A. Warczak[1] ([1]Poland, [2]USA)

P3.37

Elastic electron scattering from methane molecule in the energy range from 50-300eV

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Jelena Vuković [2]***, Karoly Tökési*** [3]***, Branko Predojević*** [2]***and Bratislav P. Marinković*** [1]

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Methane gas has been investigated widely in past years by electron collisions (see a comprehensive review of electron elastic cross sections [1]). We have done a combined experimental and theoretical study of the electron elastic differential cross sections from methane molecule (CH_4) in the intermediate energy range. The experimental setup based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron was used to measure differential cross sections. The absolute scale for the cross sections is obtained by relative-flow method using argon gas as a reference [2]. For the interpretation of the measured data we applied the partial expansion method to calculate the elastic cross sections for electron scattering from methane Fig 1. shows our theoretical results of the differential elastic electron scattering from methane molecule at 100 eV.

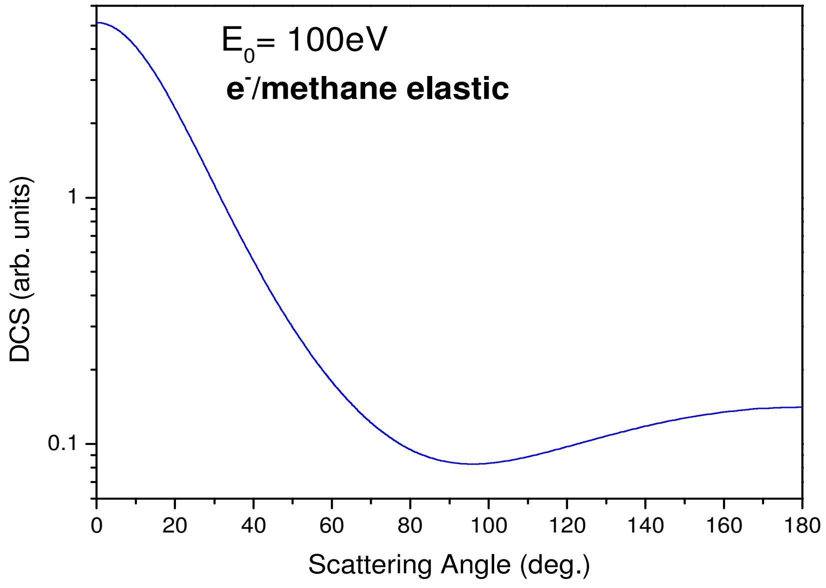

Fig. 1 Angular dependence of relative DCS for elastic electron scattering on methane molecule.

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Institute of Physics, Belgrade
University of Belgrade

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Absolute Differential Cross Sections for Electron Scattering from Anaesthetic Molecules

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We have investigated elastic electron scattering from anaesthetic molecules, halothane and sevoflurane, in the medium energy range from 50-300 eV [1]. Experiment has been performed on the UGRA apparatus [2] settled at the Institute of Physics Belgrade. The experimental setup, based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron, was used to measure differential cross sections. The absolute scale for the cross sections is obtained by relative-flow method using argon gas as a reference [3]. Absolute DCSs for elastic electron scattering from sevoflurane at 100 eV are shown in Fig.1.

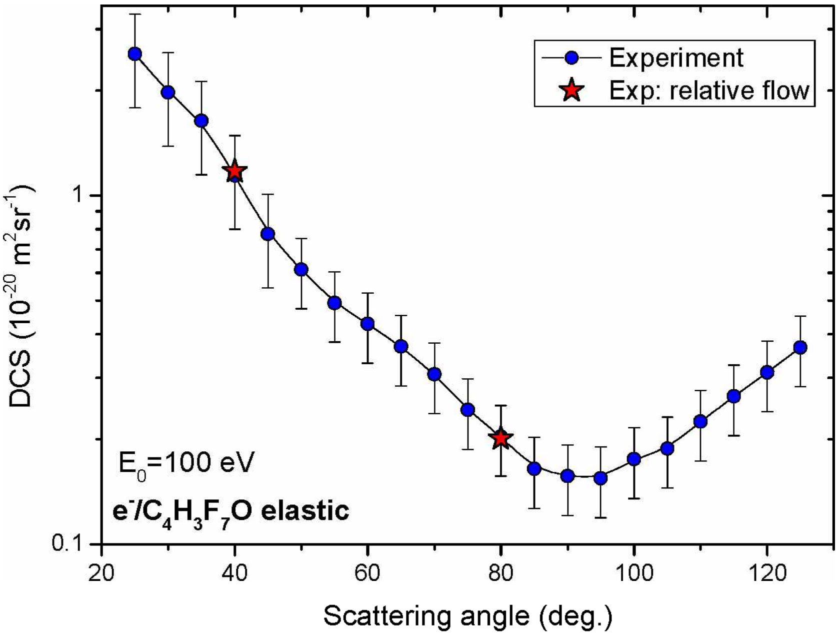

Fig.1. Angular dependence of the DCSs for elastic electron scattering from sevoflurane at 100 eV. Circles represent absolute experimental differential cross sections; stars represent absolute values obtained by relative flow method.

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[2] A. R. Milosavljević, S. Mandžukov, D. Šević, I. Čadež, and B. P. Marinković, *J. Phys. B*, **39**, (2006), 609.

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FR-117

Integral cross sections for elastic electron scattering by methane molecule

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Synopsis We have performed a combined experimental and theoretical study of electron elastic differential and integral cross sections from methane molecule (CH4) in the intermediate energy range. Data have been compared with available data sets in the literature as well as with recommended data set [Song *et al J. Phys. Chem. Ref.Data* **44** 023101 (2015)].

Methane gas has been investigated widely in past years by electron collisions [1,2]. We measured electron elastic differential cross sections (DCSs) for methane molecule (CH_4) in the energy range from 50 eV to 300 eV and angular range from 20° to 130°. DCSs were then extrapolated to zero and 180° and integrated in order to obtain the integral cross sections. The experimental setup based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron was used to measure differential cross sections.

The absolute scale for the cross sections is obtained by relative-flow method using argon gas as a reference [3]. For the interpretation of the measured data we applied the partial expansion method to calculate the elastic cross sections for electron scattering from methane.

Here we present our daa point at 50 eV and we find it in an excellent agreement with the recommended set of data [1]. At the conference we will present our data points in a full scale of electron impact energies, from 50 to 300 eV in steps of 50 eV and calculated ICS curves obtained based on IAM method and screening correction factors.

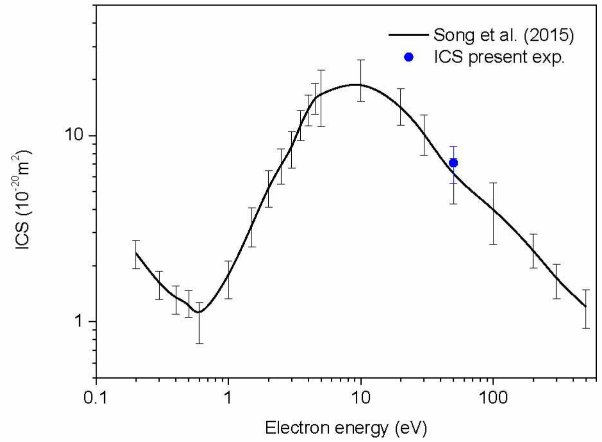

Figure 1. Energy dependence od integral cross sections for elastic electron scattering by methane molecule.

This work has been supported by the MESTD Grant #OI 171020. BPM acknowledges the grant of VAMDC consortium under Support Actions" Funding Scheme of The Seventh Framework Program. One of us KT was also supported by the National Research, Development and Innovation Office (NKFIH) Grant KH126886, and by the European COST Action CA15107 (MultiComp).

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Integral cross sections for elastic electron scattering by methane molecule

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Integral cross sections for elastic electron scattering by methane molecule

J B Maljković [1,*], J Vuković[2], K Tökési[3,4], B Predojević[2] and B P Marinković[1,†]

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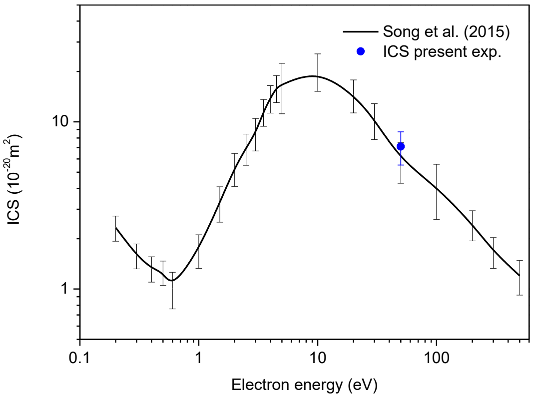

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Страна 2 - Опис истраживања

Циљеви истраживања (према достављеном плану истраживања) остварени у 2019. години имајући у виду значај, квалитет и ниво остварених резултата. ТЕМА 1. ИНТЕРАКЦИЈЕ ЕЛЕКТРОНА, ЈОНА И ФОТОНА СА АТОМИМА И (БИО)МОЛЕКУЛИМА (КОНСТИТУЕНТИМА ИЛИ АНАЛОГОНИМА ДНК МОЛЕКУЛА) РАДИ БОЉЕГ РАЗУМЕВАЊА ПРОЦЕСА РАДИЈАЦИОНОГ ОШТЕЋЕЊА. Задатак 1.1 а) На апаратури OHRHA (Omicron High Resolution Hemispherical Analyser) измерени су спектри избачених електрона аутојонизационих стања и Coster-Kronig прелаза у атому Ar, а публиковани у међународном часопису [P18. Energy analysis of ejected electrons in the region of the Ar L1-¬L2,3M Coster-Kronig transitions (25-56 eV) induced by electron impact, J. Electron Spectrosc. 237, 146898 (2019) 6pp]. б) На апаратури ESMA завршена су и публикована мерења диференцијалних пресека за еластично расејање електрона при упадним енергијама електрона од 10-100 eV на атому Zn [P12. Experimental and theoretical cross sections for elastic electron scattering from zin, Phys. Rev. A 99, 062702 (2019) 10pp]. Задатак 1.2 (руководилац задатка др Јелена Маљковић): а) Изврешена су мерења еластичног расејања електрона на молекулу три-етил-фосфату. Резултати су обрађени и публиковани [P03. Elastic electron scattering cross sections for triethyl phosphate molecule at intermediate electron energies from 50 to 250 eV, Eur. Phys. J.D 73, 27 (2019) 5pp]. б) Прелиминарна мерења еластичног расејања електрона на молекулу метана су представљена на престижним међународним конференецијама ECAMP13 и XXXI ICPEAC [CI08. Integral cross sections for elastic electron scattering by methane molecule; CI01. Elastic electron scattering from methane molecule in the energy range from 50-300 eV] в) У оквиру пост доктората у сарадњи са колегама из Прага обављен је рад о дисоцијативној јонизацији молекула флуоронитрила [O02 Phys. Chem. Chem. Phys. 21(30) 16451-16458 (2019)]. Задатак 1.3 Изучавана је теорија судара тешких честица: а) Публикован је рад у коме је примењена динамичка адијабатска теорија судара у опису атома водоника у s-стању [P05. Classical representation for hydrogen atom in s-states, Quantum Stud.: Math. Found. 6(2) 225-233 (2019)]. б) (руководилац задатка др Ненад Милојевић): Истраживан је парцијални и укупни пресек за захват електрона из К-љуске вишеелектронских мета од стране потпуно огољених пројектила. Написан је и публикован прегледни рад на ову тему у реномираном часопису. [P15. State-selective and total cross sections for electron capture from the K-shell of multi-electron atoms by fully stripped projectiles. At. Data Nucl. Data Tables, (2019) 18pp]. ТЕМА 2. ИНТЕРАКЦИЈЕ СА ПОВРШИНАМА НА НАНОМЕТАРСКОЈ СКАЛИ (НАНОКАПИЛАРЕ, НАНОТАЧКЕ) КОЈЕ ВОДЕ ФУНЦИОНАЛИЗАЦИЈИ МАТЕРИЈАЛА ИЛИ МОДИФИКАЦИЈИ НАНОФИЛМОВА. Задатак 2.1: (руководилац задатка др Милош Ранковић): Завршена тематика. Задатак 2.2 а) (руководилац задатка др Маја Рабасовић): Извршена су мерења оптичких особина прашкастих нано материјала (Sr2CeO4:Eu; GdVO4:Sm; Gd2Zr2O7:Eu; CaWO4:Nd),као и апконверзионог материјала(Gd2O3:Er,Yb). Могућности примене материјала YVO4:Eu3+ за мерења промене температуре су публиковани [P22. J. Phys. D: Appl. Phys. 53, 015106, 10pp, online 1st Oct. 2019]. Резултати анализе и карактеризације материјала CdSe/ZnS-PMMA публиковани су у радову [P17. Optical properties CaWO4:Nd3+/PMMA composite layered structures, Opt. Mater. 96, 109361 (2019) 8pp]. Оптичке особине материјала CaWO4:Nd су представљене у раду [P11. Optical properties and fluorescence of quantum dots CdSe/ZnS-PMMA composite films with interface modifications, Opt. Mater. 92, 405-410 (2019)]. б) Настављено је изучавање ласерски индукованог пробоја и посматрани различити временски размаци узорковања [P01. Laser-Induced Plasma Measurements Using Nd:YAG Laser and Streak Camera: Timing Considerations, Atoms, 7(1), 6 (2019) 12pp]. в) Испитивана је локализација електрона у двоелектронским квантним тацкама у зависности од јачине спољашњег магнетног поља и веза са квантном преплетеношћу најнижих стања и публикован је рад. [P19. Effect of the magnetic field on electron density distributions in two-electron quantum dots. J. Phys. A. Math. Theo. 52, 435303 (2019) 21pp]. 2.3 Настављена је обрада резултата TiO2 мемристора добијених FEBID техником. ТЕМА 3. ФОТОПРОЦЕСИ ВЕЗАНИ ЗА ИНТЕРАКЦИЈЕ ЛАСЕРСКОГ И СИНХРОТРОНСКОГ ЗРАЧЕЊА СА АТОМИМА, ЈОНИМА И (БИО)МОЛЕКУЛИМА. Задатак 3.1 а) Интеракција ласерског зрачења са биомолекулима (руководилац задатка др Маја Рабасовић): Настављено је изучавање временски разложених луминесцентних спектара алкалоида биљке руса [CI10. Nonlinear microscopy and time resolved fluorescence spectroscopy of Chelidonium majus L. Proc. PHOTONICA2019]. б) Интеракција синхротронског зрачења са (био)молекулима (руководилац задатка др Сања Тошић): Проучавани су могући механизами фрагментације молекула као директне последице апсорпције X зрачења помоћу подесивог синхротронског зрачења у комбинацији са различитим експерименталним техникама (PES, XPS, NEXAFS, PEPICO, PIPICO, масена спектрометрија) на различитим молекулима: i) нитроимидазолима [P10. Radiation Damage Mechanisms of Chemotherapeutically Active Nitroimidazole Derived Compounds, Front. Chem. 7, 329 (2019) 14pp: P06. Core shell investigation of 2-nitroimidazole, Front. Chem. 7, 151 (2019) 13pp]; ii) Титанијум-изо-пропоксид (органометалик, прекурсор за хемијску депозицију и ФЕБИД технику високе резолуције која омогућава стварање и уређивање наноструктурних материјала) [CI13. Photo-induced fragmentation of the titanium (IV) iso-propoxide molecule, VEIT 2019: CI12. Inner-shell spectroscopy of titanium (IV) iso-propoxide, PHOTONICA2019]. Ова истраживања су представљена и на уводном предавању у оквиру прве европске радионице корисника синхротрона одржане у Београду ESUO Organization [IT02. Core Shell Investigation and Radiation Damage Mechanisms of Nitroimidazole Compounds studies at the Gasphase Beamline @ Elettra, Photonica 2019 and 1st ESUO Regional Meeting, Belgrade, 28.08.2019] Задатак 3.2 (руководилац задатка др Предраг Коларж): Истражена ефективна доза озрачености појединих делова Балкана [O01. Effective Doses Estimated from the Results of Direct Radon and Thoron Progeny Sensors (DRPS/DTPS), Exposed in Selected Regions of Balkans, Radiation

Subject **Fwd: MD-GAS COST Action: invited talk**
From Jelena Maljkovic <jelenam@ipb.ac.rs>
To Jelena Maljkovic <jelenam@ipb.ac.rs>
Date 2022-04-11 13:48

-------- Original Message --------
Subject: MD-GAS COST Action: invited talk
Date: 2019-12-18 11:52
From: Alicja DOMARACKA <domaracka@ganil.fr>
To: <jelenam@ipb.ac.rs>

Dear Jelena Maljkovic,

On behalf of the Scientific Organizing Committee I would like to invite you to give a talk with the tentative title _Elastic electron scattering processes_ at the first General Meeting of the COST Action: MD-GAS (Molecular Dynamics in the GAS-phase). The meeting will be held at the GANIL facility in Caen, France, February 18-21, 2020. See https://www.cost.eu/actions/CA18212/#tabs|Name:overview [1] for more information about this new COST Action, which started on November 12, 2019. Invited talks will be 25 min+5 min for questions.

Note that there is no registration fee. Further information will soon be available on the meeting website: https://md-gas.sciencesconf.org

Given the very short time to meeting, we kindly ask for your definite decision within 7 calendar days.

In case of a positive response, please also provide the title of your talk.

We look forward to hearing from you soon.

Best regards,

Alicja Domaracka,

on behalf of the Scientific Organizing Committee

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****
Alicja Domaracka (CNRS)
CIMAP - Centre de Recherche sur les Ions, les Matériaux et la Photonique
UMR 6252 (CEA - CNRS - ENSICAEN - Université de Caen Normandie)
CIMAP - GANIL Bd H. Becquerel - BP 5133 - 14070 CAEN Cedex 5 FRANCE
Tél : +33 (0) 2 31 45 45 03
Fax : +33 (0) 2 31 45 47 14
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[1] https://www.cost.eu/actions/CA18212/#tabs|Name:overview

--
Institute of Physics Belgrade
Pregrevica 118, 11080 Belgrade, Serbia
http://www.ipb.ac.rs/

Subject **COST Action CA20129: Update of Working Group Assignment**
From COST Association Notification <noreply@cost.eu>
To Jelena Maljkovic <jelenam@ipb.ac.rs>
Date 2022-02-10 16:11

webmail

cost
EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

Dear Dr Jelena Maljkovic,

This is to inform you that your Working Group assignment has been updated. You are currently assigned to the following Working Groups of COST Action CA20129:

WG1: 1. Irradiation- and chemistry-driven multiscale phenomena
WG4: 4. Training, dissemination and outreach

If you need further information, please contact the Action.

Best regards,

COST Association

COST Association | Avenue du Boulevard-Bolwerklaan 21
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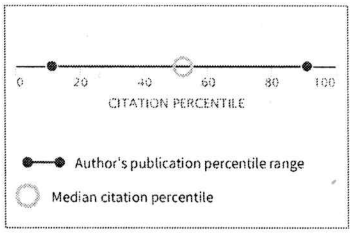

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Published 2022 | INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES
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Elastic Electron Scattering from Methane Molecule in the Energy Range from 50-300 eV
Vukalovic, Jelena ; Maljkovic, Jelena B. ; (...); Marinkovic, Bratislav P.
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Integral cross sections for elastic electron scattering by methane molecule
Maljkovic, J. B. ; Vukovic, J. ; (...); Marinkovic, B. P.
Published 2020 | 31ST INTERNATIONAL CONFERENCE ON PHOTONIC, ELECTRONIC AND ATOMIC COLLISIONS (ICPEAC XXXI)
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Elastic electron scattering cross sections for triethyl phosphate molecule at intermediate electron energies from 50 eV to 250 eV
Maljkovic, Jelena B. ; Vukovic, Jelena ; (...); Marinkovic, Bratislav P.
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Electron transmission through a steel capillary
Maljkovic, J. B. ; Borka, D. ; (...); Tokesi, K.
Published 2018 |
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Elastic electron differential cross sections for argon atom in the intermediate energy range from 40 eV to 300 eV
Rankovic, Milos Lj. ; Maljkovic, Jelena B. ; (...); Marinkovic, Bratislav P.
Published 2018 | EUROPEAN PHYSICAL JOURNAL D
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Dissociative electron attachment to coordination complexes of chromium: chromium(0) hexacarbonyl and benzene-chromium(0) tricarbonyl
Kopyra, Janina ; Maciejewska, Paulina ; Maljkovic, Jelena
Published 2017 | BEILSTEIN JOURNAL OF NANOTECHNOLOGY
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Study of electron transmission through a platinum tube
Milosavljevic, A. R.; Rankovic, M. Lj.; (...); Tokesi, K.
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Study of electron transmission through a metallic capillary
Milosavljevkic, A. R.; Rankovic, M. Lj.; (...); Tokesi, K.
Published 2015 | JOURNAL OF PHYSICS CONFERENCE SERIES

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Absolute differential cross sections for elastic electron scattering from small biomolecules
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Published 2014 | 27TH SUMMER SCHOOL AND INTERNATIONAL SYMPOSIUM ON THE PHYSICS OF IONIZED GASES (SPIG 2014)

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Electron impact excitation of methane: determination of appearance energies for dissociation products
Danko, M.; Orszagh, J.; (...); Matejcik, S.
Published 2013 | JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

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Absolute cross sections for electron scattering from furan
Maljkovic, J. B.; Blanco, F.; (...); Milosavljevic, A. R.
Published 2012 | JOURNAL OF CHEMICAL PHYSICS

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Elastic electron scattering from formamide molecule
Maljkovic, J. B.; Blanco, F.; (...); Milosavljevic, A. R.
Published 2012 |
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Absolute cross sections for elastic electron scattering from methylformamide
Maljkovic, J. B.; Blanco, F.; (...); Milosavljevic, A. R.
Published 2012 | PHYSICAL REVIEW A

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Absolute differential cross sections for elastic scattering of electrons from pyrimidine
Maljkovic, J. B.; Milosavljevic, A. R.; (...); Marinkovic, B. P.
Published 2009 | PHYSICAL REVIEW A

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Absolute cross sections for elastic electron scattering from 3-hydroxytetrahydrofuran
Milosavljevic, A. R.; Blanco, F.; (...); Marinkovic, B. P.
Published 2008 | NEW JOURNAL OF PHYSICS

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RELATIVE ANGLE-DIFFERENTIAL CROSS SECTIONS FOR ELASTIC ELECTRON SCATTERING FROM PYRIMIDINE
Maljkovic, J. B.; Milosavljevic, A. R.; (...); Marinkovic, B. P.
Published 2008 | 24TH SUMMER SCHOOL AND INTERNATIONAL SYMPOSIUM ON THE PHYSICS OF IONIZED GASES, CONTRIBUTED PAPERS

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Optical and electron spectrometry of molecules of biological interest
Marinkovic, B. P.; Milosavljevic, A. R.; (...); Pejcev, V.
Published 2007 | ACTA PHYSICA POLONICA A

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Cross section data for electron collisions in plasma physics
Marinkovic, B. P.; Pejcev, V.; (...); Maljkovic, J. B.
Published 2007 | JOURNAL OF PHYSICS CONFERENCE SERIES

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Комисија за стицање научних звања

Број:660-01-0001/570
15.07.2019. године
Београд

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На основу члана 22. став 2. члана 70. став 4. и члана 86. ст. 1. и 2. Закона о научноистраживачкој делатности ("Службени гласник Републике Србије", број 110/05 и 50/06 – исправка, 18/10 и 112/15), члана 3. ст. 1. и 3., члана 32. став 1., члана 35. став 1. и члана 40. Правилника о поступку, начину вредновања и квантитативном исказивању научноистраживачких резултата истраживача ("Службени гласник Републике Србије", број 24/16, 21/17 и 38/17) и захтева који је поднео

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ОДЛУКУ
О СТИЦАЊУ НАУЧНОГ ЗВАЊА

Др Јелена Маљковић

стиче научно звање

Научни сарадник

Реизбор

у области природно-математичких наука - физика

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ПРЕДСЕДНИК КОМИСИЈЕ

Др Ђурђица Јововић,
научни саветник

МИНИСТАР

Младен Шарчевић