Physics and Chemistry of Solved Electron

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Outline

- What is “solvated electron” ?
- Localization of excess electrons in condensed molecular media
- Experimental detection and spectroscopic manifestations of hydrated electron
- Solvated electrons in other molecular liquids and glasses
- Models of solvated electron
- Solvation dynamics: “digger” or “seeker” ?
- Thermodynamic and transport properties of e^-_{aq}
- Solvated electron as a chemical reagent
- Kinetics and mechanism of reactions solvated electron
- Excess electrons in ionic liquids
- Some implications and applications

What is “solvated electron” ?

- Solvated electron – **a solvent-bound state of excess electron in liquid or glassy media, which is often treated as an anion-like “chemical entity”**
- Known for more than 100 years: blue-coloured solutions of alkali metals in liquid ammonia

first observation: **W. Weyl (1864);**

hypothesis of “electron equilibrium”: **C. Kraus (1908)**

$$M + aNH_3 \rightleftharpoons [M(NH_3)_{a-x}]^+ + e^-(NH_3)_x$$

- **Honored 50 years ago**: observation of hydrated electron in 1962 – listed among top 50 discoveries in chemistry of the 20th century
- **Still “unbelievable”...(**continuos critisism, sometimes, even ignorance)
- **Very well studied**: more than 2000 papers, ca. 1500 kinetic constants
- **Still not completely understood, a “hot” topic** (see, e.g. Marsalek et al., *Acc. Chem. Res*., 2012; four papers only in *Science* during last two years)

Why do we care about solvated electron ?

- Basic understanding of electron transport and localization in condensed media, related to molecular electronics, chemical physics and biophysics
- One of the key species in radiation chemistry, photochemistry and photoelectrochemistry in solutions
- Preparative chemistry and environment-friendly technologies: unique chemical reagent (clean and very efficient reducing agent)
- Unique probe for microscopic properties of disordered media (including confined environment, organized assemblies and interfaces) – electric, optical and magnetic response

Generation of solvated electron

- **1. High-energy irradiation (fast electrons, X-rays, etc.):**
  - $M \rightarrow M^{+\cdot} + e^-_{qf}$ ($e^-_{qf} \rightarrow e^-_{loc} \rightarrow e^-_s$) *(universal)*
- **2. Photoionization of solutes with low** IP (e.g.,$Fe(CN)_6^{4-}$, amines, SO_3^{2-} (λ = 220 – 500 nm)
- 3. **Heterogeneous photoelectron emission from metals (electron photoinjection from electrode into solution)**
- **4. Heterogeneous chemical reactions:**
  - $Na + NH_3 \leftrightarrow Na^+ + e^-_s$
  - $Na(Hg) + H_2O \rightarrow Na^+ + e^-_{aq}$
  - $U^{3+} + H_2O \rightarrow U^{4+} + e^-_{aq}$

…

Excess electrons in condensed dielectrics

- **Избыточные (*excess*) электроны** – неравновесные носители, инжектированные в диэлектрик (путем фотоионизации, электронного удара и проч.)
- Для ***«квазисвободных»*** избыточных электронов (e^-_{qf}), не обладающих избыточной кинетической энергией:

$$E = V_0$$

(V_0 – основной уровень электрона в среде – отсчет от вакуума)

Методы определения V_0

- 1) по разности работ выхода электрона из металла в вакуум и в жидкость:

$$V_0 = \varphi_{liq} - \varphi_{vac}$$

- 2) по разности ПИ в газе и жидкости:

$$V_0 = I_g - I_{liq} - P^+$$

$$P^+ = (e^2/8\pi\varepsilon_0)(1 - \varepsilon_\infty^{-1})$$

V_0 values and electron mobility in dielectric liquids

Medium	***V_0, eV***	***u,*** см^2 /(V· s)*
Helium	1.0	0.02
Neon	0.6	0.002
Ethane	~0.2	0.014
n-Pentane	~0	0.15
n-Hexane	~0	0.09
Methane	***~0***	***400***
Benzene	- 0.14	0.1
Neopentane	- 0.43	70
Tetrametylsilane	- 0.6	100
Xenon	- 0.65	2200
Ethanol	*- 0.65*	*0.0003*
Water	*- 1.3 (?)*	*0.002*

*u = v/E, в литературе чаще обозначается как μ

E_A = 0.02 – 0.5 эВ (для метана $E_A < 0$)

Electron autolocalization in a dielectric lattice. Polarons

- **Polaron** – *квазичастица* – движущийся электрон плюс индуцированное им поляризационное поле в кристалле. Поляризация вызывает *деформацию кристаллической решетки* (образуется «*фононное облако*», сопровождающее электрон*)*
- Поляризационное поле «тормозит» электрон: **m* > m**

- **Теория полярона**: ***С.И. Пекар***, Л.Д. Ландау; H. Frölich
- **Weak coupling case** (α **<<1** – ***константа Фрёлиха***, характеризующая электрон-фононное взаимодействие):

$$\alpha = \frac{\sqrt{2}e^2 m^{1/2}}{2\omega_l^{1/2}\;{}^{3/2}}(\varepsilon_\infty^{-1} - \varepsilon^{-1}) \qquad \frac{m^*}{m} \approx 1 + \frac{\alpha}{6} + 0.0236\alpha^2.$$

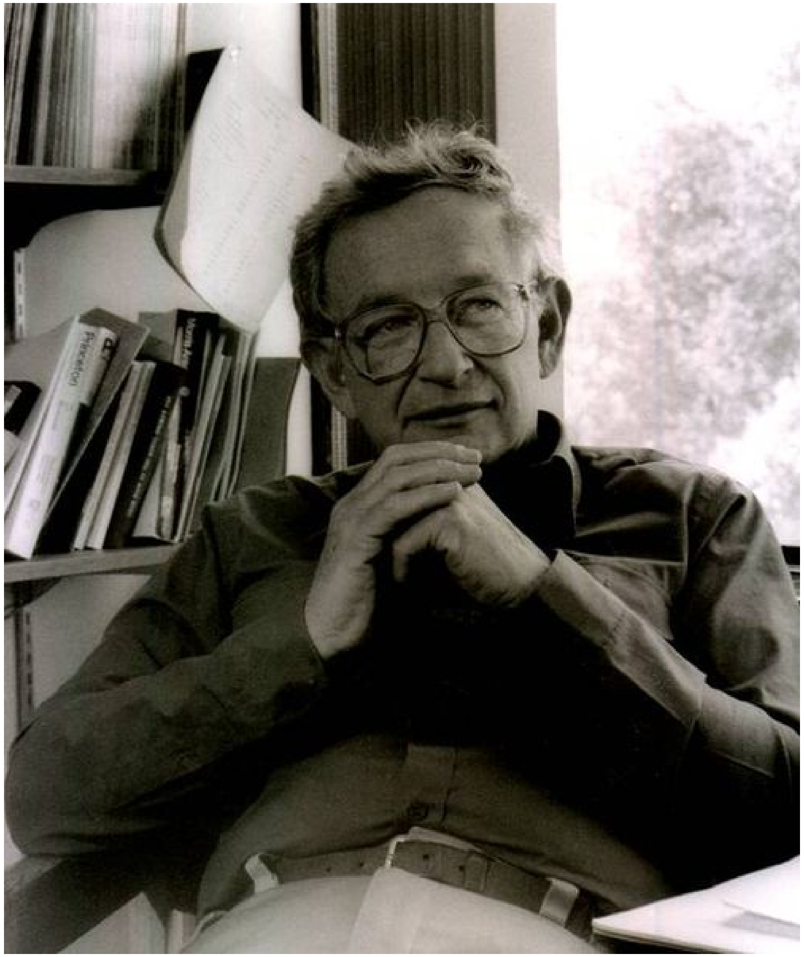
- **Strong coupling case** ***(*α *≥ 5)***: **self-localization** *(**r_l** ~ 1 нм)*

$$\frac{m^*}{m} \approx 0.023\alpha^4$$

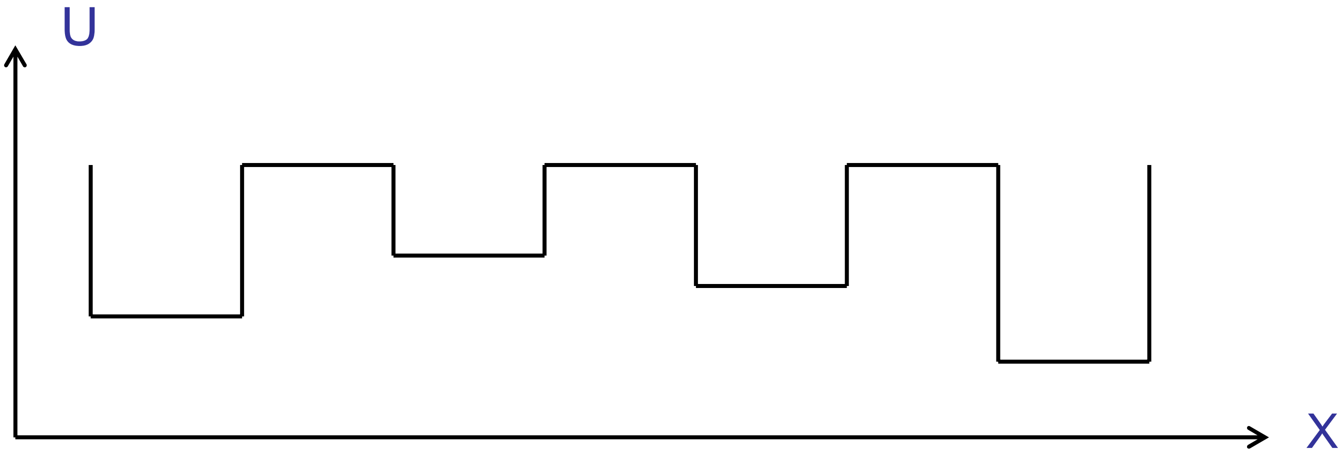
- Поляроны могут захватываться *дефектами*
- Понятие «полярона», введенное для ионных кристаллов, распространено на молекулярные среды, полимеры, низкоразмерные системы…

Anderson localization in disordered media

- ***P.W. Anderson*** (1958; Nobel prize, 1977): в среде с пространственными неоднородностями *распространение бегущей волны невозможно* → формирование *стоячей волны, сконцентрированной в определенной области* ***(локализация)***
- Применимо к аморфным металлам, полупроводникам, ***диэлектрикам***



Electron energy in a disordered medium



Простейшая модель одномерной андерсоновской решетки («вертикальный беспорядок»

***Трехмерная решетка**: ε_g – **порог подвижности** (для диэлектриков $\varepsilon_g < \varepsilon_F$)*

- *Предельное* распределение *плотности вероятности* (t → ∞), если *энергия принадлежит области локализованных состояний*

ρ(R) ~ const при R<<L **ρ(R) ~ exp(-R/L) при R>>L**

- Андерсоновский (неупорядоченный) диэлектрик:

$\sigma = 0$ при $T = 0$ K; «*прыжковый*» механизм при $T > 0$

Molecular localization: excess electron capture

- Excess electrons can be captured by solvent molecules or impurities with *positive effective electron affinity*

$$M\ (s) + e^-_{qf} \rightarrow M^{-\cdot}(s)$$

- $O_2\ (s) + e^-_{qf} \rightarrow O_2^{-\cdot}(s)$ (1)
- $CO_2\ (s) + e^-_{qf} \rightarrow CO_2^{-\cdot}(s)$ (2)
- $CH_3COCH_3\ (s) + e^-_{qf} \rightarrow CH_3COCH_3{}^{-\cdot}(s)$ (3)

- *The role of solvation:* Possible capture of electron by molecules with slightly negative gas-phase EA (ex. 3) $|\Delta G_s(M)| << |\Delta G_s(M^{-\cdot})|$

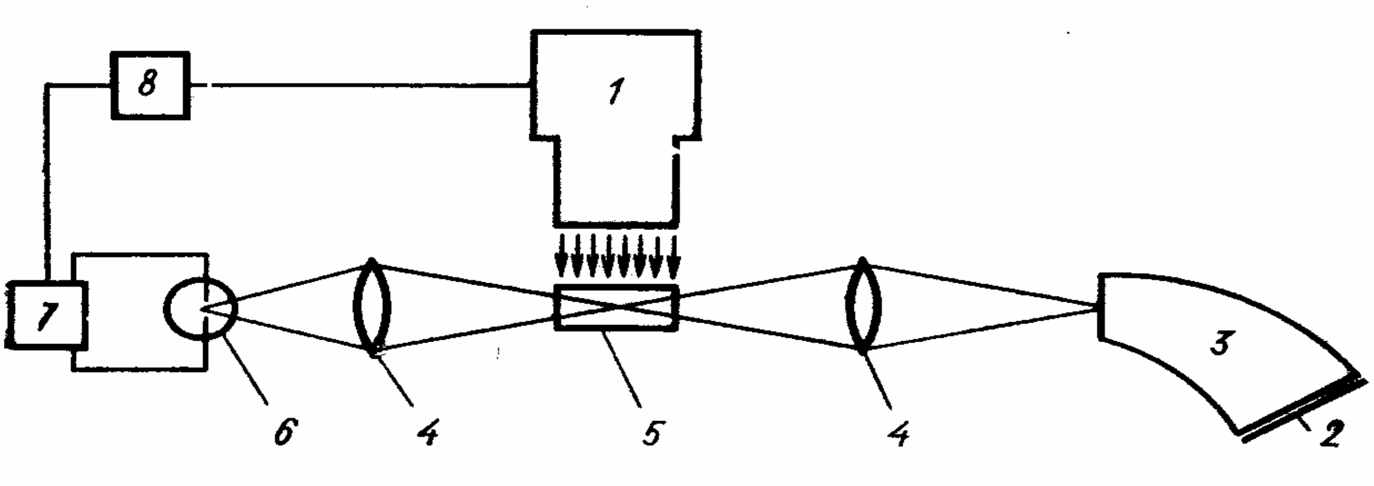
- Capture by dimers or clusters:

$$M_n\ (s) + e^-_{qf} \rightarrow M_n{}^{-\cdot}(s)$$

Localization of excess electrons: preliminary conclusions

- Excess electrons become localized in dielectric crystals and disordered molecular media (liquids, glasses) → sharp drop in electron mobility
- Different mechanisms may be responsible for electron localization in molecular media

Pulse radiolysis



The scheme of experimental set-up used by Boag and Hart (1962)

: *1* – ускоритель электронов, *2* – фотопластина, *3* – спектрограф, *4* – линза, *5* – ячейка, *6* – импульсная лампа, *7* – блок питания лампы, *8* – блок регулируемой задержки)

Pulse duration 2 μs, resolution 5 μs; spectral range 300 – 880 nm

The up-to-date level (*pulse-probe*) :
Pulse duration 10 ps, resolution 1 ps
(Orsay, France, 2006)
Pulse duration 100 fs, resolution 250 fs *(Osaka, Japan, 2009)*

Discovery of the hydrated electron

- ***J.W. Boag, E.J. Hart (1962):***

Detection of optical absorption in the *red region **(λ_{max} ~ 720 nm) upon irradiation of liquid water with fast electrons***

Assignment: hydrated electron (e^-_{aq}) [τ ~ 20 μs]

$$H_2O \;\text{--/}\backslash\text{/}\backslash\text{-}\!\rightarrow H_2O^{+\cdot},\ H_2O^{*},\ e^-$$

$$H_2O^{+\cdot} + H_2O \rightarrow H_3O^+ + OH^{\cdot}$$

$$e^- \rightarrow e^-_{aq}$$

$$H_2O^{*} \rightarrow H^{\cdot} + OH^{\cdot} \quad (?)$$

Arguments:

(1) Spectroscopic ($H^\cdot$, $^\cdot OH$, H_2O_2, H_3O^+, OH^-) *cannot absorb in the red region*

(2) Chemical (absorption is suppressed in the presence of elctron scavengers : O_2, CO_2,N_2O)

J.W. Boag, E.J. Hart, *Nature*, 1963, **197**, 45; independently J.P. Keene, *Nature*, 1963, **197,** 47

Spectroscopic properties of e^-_{aq}

Hydrated electron: ***z = -1, S = ½***

(a charged paramagnetic species)

- ***Optical spectrum (298 K):***

  λ_{max} = 715 nm (E_{max} = 1.73 eV)

  ε_{max} = 1.85 · 10^4 M $^{-1}$см$^{-1}$

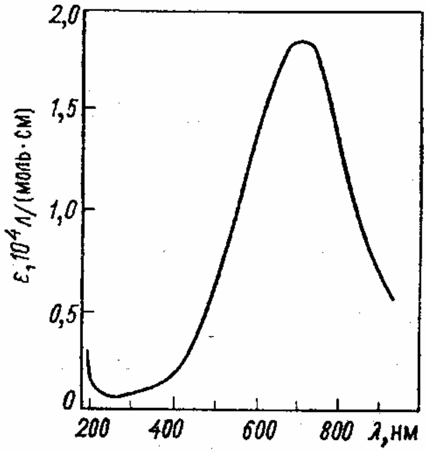
  $\Delta E_{1/2}$ = 0.93 eV

  F ≈ 0.7 (allowed transition)*

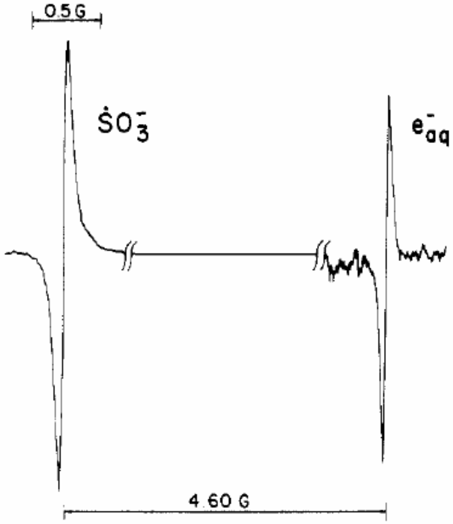
- ***EPR signal (283 K, lquid)***

  Sinflet ***g* = 2.00043** (close to g_e)

  ΔB < 0.01 mT (dynamic narrowing)



Optical spectrum of **e^-_{aq}** *at 298 K*



EPR spectrum of **e^-_{aq}** *at 296 K*
(Jeevarandan & Fessenden J. Phys. Chem., 1989, ***93****, 3511) – in situ photolysis of sulphite anion*
Independent of generation method

)F = 4.315 * 10^{-9} $\int \varepsilon d\nu$ ($\nu = 1/\lambda$)

Solvated electrons in other molecular media

Medium	***λ_{max} ,nm***	***E_{max} , eV***	***μ, D***	***ε***
Methanol	630	1.96	1.67	33.6
Ethanol	700	1.77	1.70	25.1
2-Propanol	820	1.5	1.65	19
EG	580	2.1	2.28	38
THF	~2100	~0.6	1.63	7.3
n-Hexane	*> 1600*	*< 0.8*	*0.08*	*1.89*
Ammonia (225 K)	1400	0.89	1.44	22
Water	*715*	*1.73*	*1.83*	*80*

E_{max} – optical trap depth

No direct correlation between E_{max} и and molecular (dipole moment) or macroscopic (ε_{cm}) properties of liquids

Solvated (trapped) electrons in molecular glasses (77 K)

$\eta_g / \eta_l \sim 10^{15} - 10^{30}$

$\tau\ (e^-_{tr}) \rightarrow \infty$

Medium	***λ_{max} , nm***	***E_{max} , eV***	***ΔB,мT (EPR)***
Methanol	520	2.38	~1.4
Ethanol	540	2.28	~1.2
2-Propanol	645	1.92	~1.0
EG	500	2.41	~1.5
2-MTHF	1250	1,0	0.4
3-Methylpentane	1650	0.75	0.3
*Water (ice)**	*630*	*1.96*	*~1.5*

Spectral properties of e^-_s и e^-_{tr} are similar. E_{max} (e^-_{tr}) > E_{max} (e^-_s) (ΔE ~ 0.2–0.4 eV). ***ΔB increases with increasing*** **E_{max} (determined by the HFC constants of unpaired e^- with matrix protons)**

* *в присутствии инертных солей*

The structure of solvated electron: models

- Классы моделей:
- 1. Continual (связь с макроскопическими характеристиками непрерывной среды): *поляронная модель, модель полости*.
- 2. Configuration-continual (semi-contnual)
- 3. Molecular dynamics simulation

Экспериментальные данные для верификации моделей:

- энергия связи (оптическая глубина ловушки)

- оптический спектр поглощения (форма)

- ? - *магнитно-резонансные характеристики (ЭПР) – наиболее чувствительны к геометрическим деталям*

Polaron model (before 1960)

- ***A. S. Davydov*** (1948,based on polaron theory as formulated by Pekar)

- Potential: $V = -\beta e^2/r$ $(\beta = \varepsilon^{-1}_{\infty} - \varepsilon^{-1})$
- Optical transition: $1s \rightarrow 2p$

$$E_{\max}(\text{эВ}) = \Delta E = E_{2p} - E_{1s} \approx 1.93\beta^2 \frac{m^*}{m}$$

- Optimum values **m*/m**: **1.5** (ammonia); **2.7** (water) (realistic*?)*
- (-) no clear physical interpretation of m*
- (-) no explanation of $E_{max}(T, p)$
- (-) the spectral shape cannot be interpreted

unsatisfactory

Cavity model

Jortner et al. (1964): электрон локализуется в «полости» радиусом R_0

- $V = -\beta e^2/r \quad (r > R_0)$

  $V = -\beta e^2/R_0 \quad (r < R_0)$

Fitting: energy of the 1s → 2p optical transition

E_{max} increases with increasing R_0

- **Ammonia** ***R_0 = 0.30 – 0.34 nm*** (estimated from volume expansion coefficient upon dissolution of alkali metals in ammonia)
- **Water** ***R_0 = 0.14 – 0.15 nm (optimized)***

- *Qualitative explanation for e^-_{aq} :*
- **$dE_{max}/dT = -2.9 \cdot 10^{-3}$ эВ/ К** (<0, thermal expansion of the cavity)
- **$dE_{max}/dp = 8 \cdot 10^{-7}$ эВ/ кПа** (>0, baric confinement)
- Correlation between E_{max} and с ΔB

Microscopic sense ?

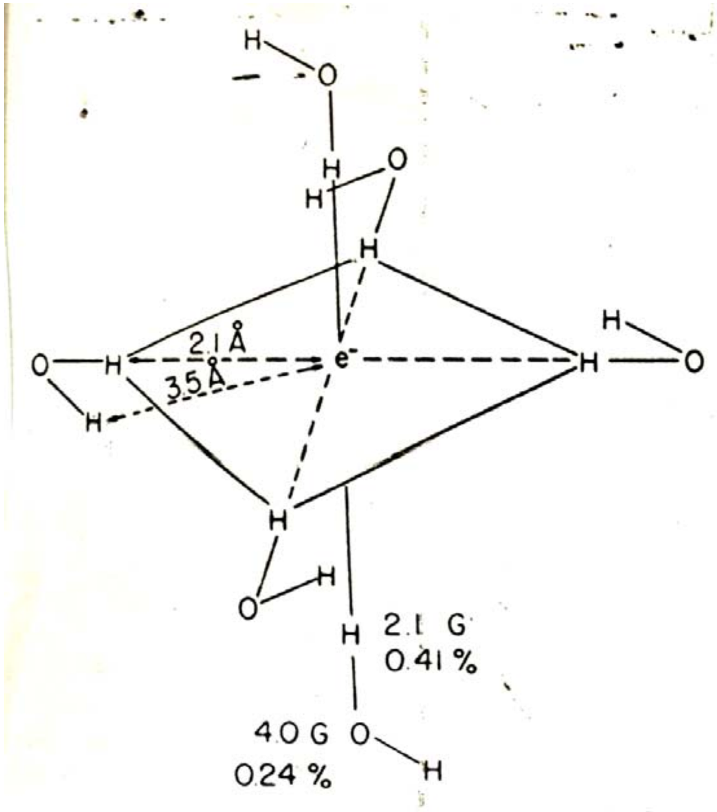
Configuration-continual (geometrical) models

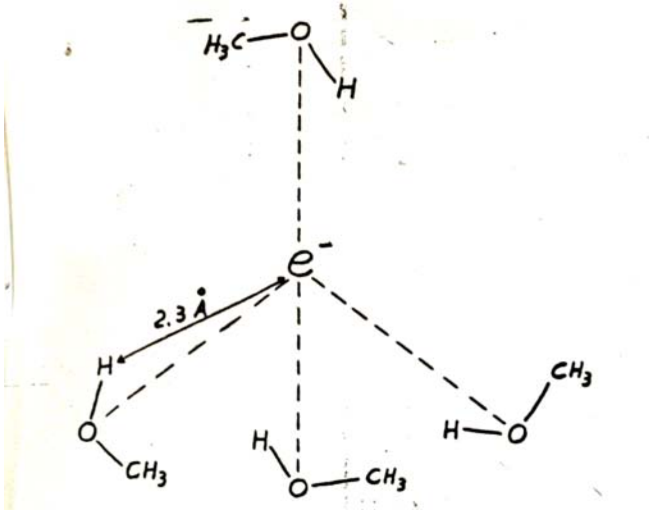
- Specific geometrical configuration of the first co-ordination sphere (“trap”) + continuum nedium среда: **$(X_n^{-\cdot})_{solv}$**

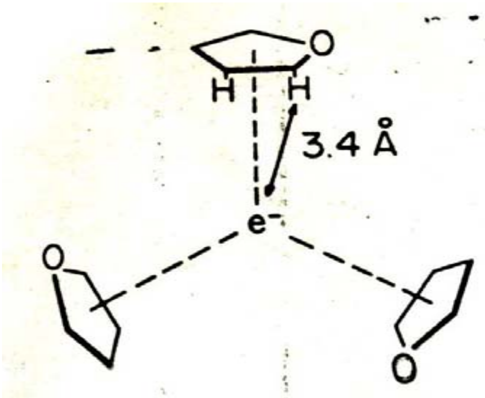
- Arguments:
  - Observation of metastable negatively charged clusters $(H_2O)_n^{-\cdot}$ (n > 4) in the gas phase
  - Results of pulsed magnetic measurements (ESEEM) in glasses

None of these arguments are directly related to the liquid phase

Geometry of e^-_{tr} in glassy matrices at 77 K as revealed by ESEEM experiment

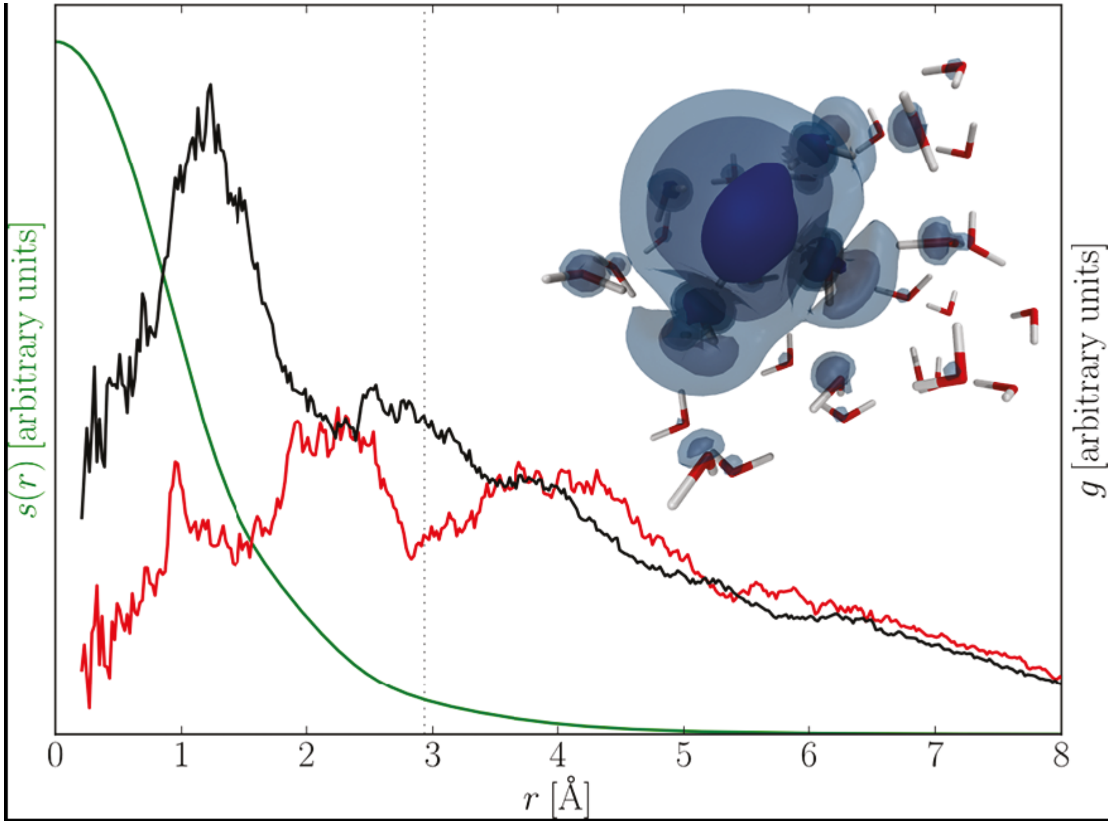






L. Kevan, Acc. Chem. Res., 1981, ***14****, 138*

Molecular dynamic simulation

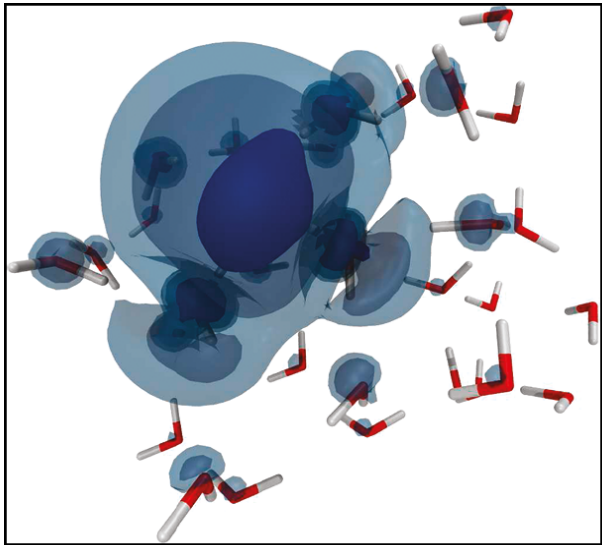


The structure of hydrated electron as revealed by ab initio MD simulation for excess electron embedded in a water cluster (n = 32) at 300 K. Radial density of the excess electron averaged over the angular variables (green) and radial distribution function of water oxygen (red) and hydrogen (black) atoms relative to the center of the excess electron from equilibrium configurations at T = 300 K.

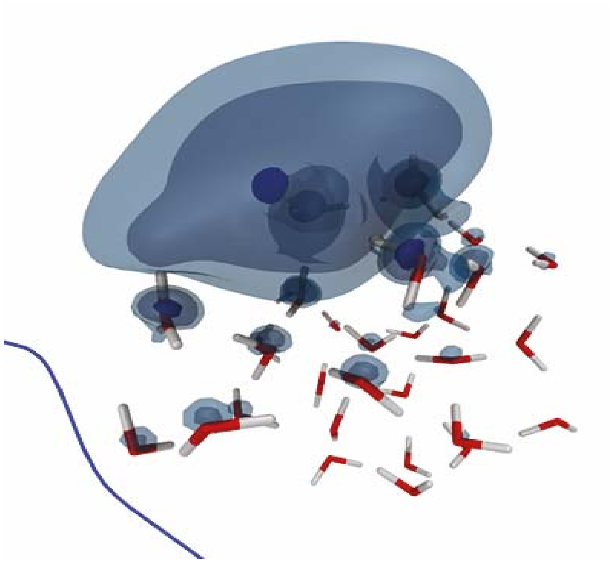
(Marasalek et al., *Acc. Chem. Res.*, 2012)

MD simulation: preliminary conclusions

Effect of temperature:



300K: cavity



30 K: "cushion-like" state ?

- A cavity model can be adopted as a *rough approximation*
- Cavity is more flexible and accessible to water molecules (as compared to those containing negative ions)
- The configuration of solvated electron at low temperature (in frozen ice) may be significantly different (?)

(Marasalek et al., *Acc. Chem. Res*., 2012)

...still far from being clear

Dynamics of electron solvation: “digger” or “seeker” ?

- ***Digger***: электрон сам «выкапывает» себе ловушку за счет ориентации молекул растворителя в сильном локальном электростатическом поле

- ***Seeker:*** электрон «ищет» подходящую ловушку (конфигурацию диполей), изначально существующую в полярной жидкости (*pre-existing trap, pre-trap*)

- First direct observation of electron solvation dynamics at low temperatures:

(J.H. Baxendale, P. Wardman, *Nature*, 1971, **230**, 449)

e^-_{loc}(IR, λ_{max}>1350 nm) → e^-_s (λ_{max}= 700 – 800 nm)

- Solvation time: ethanol τ_S = 3 ns (166 K)
- 1- propanol τ_S = 5 ns (178 K); 60 ns (152 K)
- 2-propanol: τ_S = 6 ns (186 K)
- 1-butanol : τ_S = 4 ns (184 K)

… both “digger” and “seeker” ?

$$e^-_{qf} \underset{\uparrow}{\rightarrow} e^-_{loc} \underset{\uparrow}{\rightarrow} e^-_{s}$$

seek …. dig

<u>2-nd stage</u>: “continuous shift” due to orientational polarization (“digging”) or trap-to-trap tunneling ?

Correlation between solvation time and solvent relaxation properties

Electron solvation in alcohols at 300 K (G.A. Kenney-Wallace, 1982)

Alcohol	τ_S, *ps*	τ_2, *ps**	η
Methanol	11	12	0.55
Ethanol	18	20	1.10
1-Propanol	24	22	2.00
1-Butanol	30	27	2.60
1-Octanol	45	39	8.95
1-Decanol	51	48	14.1

rotational relaxation time for monomeric molecules

$\tau_S \sim \tau_2$ ("digging" ?)

No direct correlation with viscosity

τ_S (e^-_{aq}) = 0.54 ps (Yoshida et al., 2010). No digging ?

Thermodynamical properties of e^-_{aq}

- $E^0 = - 2.87$ V
- $\Delta G^0 = -157$ kJ/ mol
- $\Delta H^0 = -136.4$ kJ/ mol
- $S^0 = 69.8$ J/ (mol· К)
- $\Delta S^0_{hydr} = 49$ J/ (mol·K)

ΔG^0 (e^-_{aq})

$e^-_{aq} + H^+_{aq} \rightarrow \frac{1}{2} H_{2\,(aq)}$

- $\frac{1}{2} H_{2\,(aq)} \rightarrow \frac{1}{2} H_{2\,(g)}$
- $\frac{1}{2} H_{2\,(g)} \rightarrow H_g$
- $H_g \rightarrow e^-_g + H^+_g$
- $H^+_g \rightarrow H^+_{aq}$

$e^-_{aq} \rightarrow e^-_g$

Transport properties of e^-_{aq}

Ionic conductivity and drift mobility:

$$\lambda^0_- (e^-_{aq}) = 185\ \text{см}^2/(\text{Ohm} \cdot \text{g-eqv})$$

(cf.: OH^-: 198; Cl^-: 70)

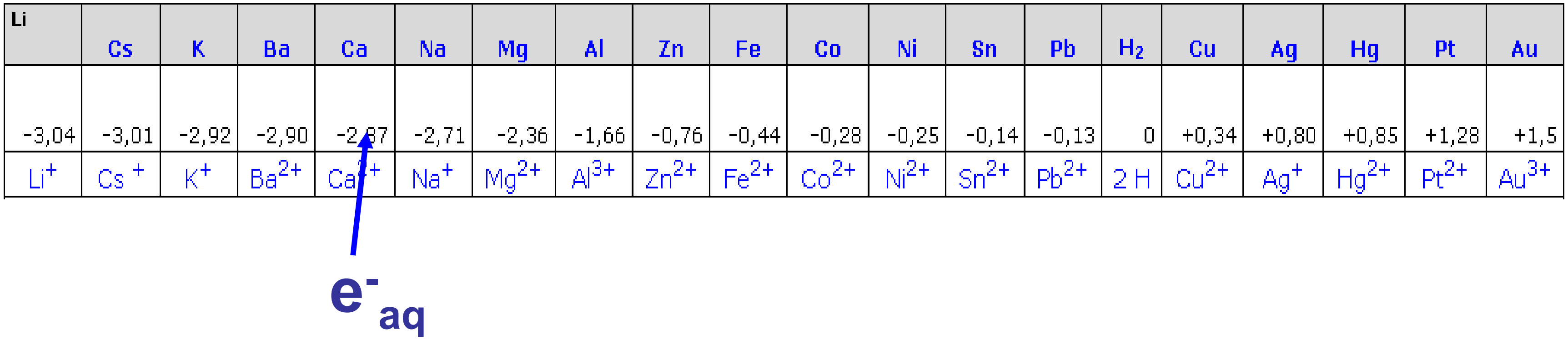
$$u_- (e^-_{aq}) = 1,92 \cdot 10^{-3}\ \text{см}^2 /(\text{V} \cdot \text{s})$$

Diffusion coefficient

$$D (e^-_{aq}) = 4.96 \cdot 10^{-5}\ \text{см}^2 / \text{s}$$

(much higher than for heavy anions →
non-classical diffusion ?)

Solvated electron as a chemical reagent



Li	Cs	K	Ba	Ca	Na	Mg	Al	Zn	Fe	Co	Ni	Sn	Pb	H_2	Cu	Ag	Hg	Pt	Au
-3,04	-3,01	-2,92	-2,90	-2,87	-2,71	-2,36	-1,66	-0,76	-0,44	-0,28	-0,25	-0,14	-0,13	0	+0,34	+0,80	+0,85	+1,28	+1,5
Li^+	Cs^+	K^+	Ba^{2+}	Ca^{2+}	Na^+	Mg^{2+}	Al^{3+}	Zn^{2+}	Fe^{2+}	Co^{2+}	Ni^{2+}	Sn^{2+}	Pb^{2+}	2 H	Cu^{2+}	Ag^+	Hg^{2+}	Pt^{2+}	Au^{3+}

e^-_{aq}

Гидратированный электрон – уникальный *«чистый» одноэлектронный восстановитель* (более эффективный, чем атом H, не дает «побочных» продуктов)

Basic reactions of e^-_{aq}

Reduction of metal cations

- $e^-_{aq} + M^{n+} \rightarrow M^{(n-1)+}$ $(k \geq k_{diff})$

$e^-_{aq} + Ni^{2+} \rightarrow Ni^+$

$e^-_{aq} + Ag^+ \rightarrow Ag^0$

$e^-_{aq} + Cu^+ \rightarrow Cu^0$

Reactions with inorganic anions

$e^-_{aq} + NO_3^- \rightarrow NO_3^{2-}$

$e^-_{aq} + MnO_4^- \rightarrow MnO_4^{2-}$

Non-dissociative attachement to neutral molecules

$e^-_{aq} + O_2 \rightarrow O_2^{-\cdot}$

$e^-_{aq} + CH_3COCH_3 \rightarrow CH_3COCH_3^{-\cdot}$

$e^-_{aq} + C_6H_6 \rightarrow C_6H_6^{-\cdot}$

Dissociative attachemnt to neutral molecules:

$e^-_{aq} + N_2O \rightarrow N_2 + O^{-\cdot}$

$e^-_{aq} + RBr \rightarrow R^{\cdot} + Br^-$

Reaction kinetics: rate constants for e^-_{aq}

Classificasion of reactions:

- \- fast (diffusion-controlled)
- \- «ultrafast»
- \- slow

Molecule or ion	*k, $M^{-1}s^{-1}$**
Cd(II)	$5.1 \cdot 10^{10}$
Ag (I)	$3.9 \cdot 10^{10}$
Cu(II)	$3.5 \cdot 10^{10}$
MnO_4^-	$3.3 \cdot 10^{10}$
Chloroform	$3 \cdot 10^{10}$
O_2	$1.9 \cdot 10^{10}$
N_2O	$9.1 \cdot 10^{9}$
CO_2	$7.7 \cdot 10^{9}$
Acetone	$6.6 \cdot 10^{9}$
Benzene	$1.2 \cdot 10^{7}$(pH=11- 13)
Methanol	$< 10^4$

*pH = 7, unless otherwise stated

Diffusion-controlled reactions of e^-_{aq}

$$k_{dif} = \frac{4\pi r D N_A}{1000} (t \to \infty)$$

$r = R_A + R_B; D = D_A + D_B$

(reactions with neutrals)

$$k_{dif} = \frac{4\pi r_{eff} D N_A}{1000} \qquad r_{eff} = [\int_r^\infty \frac{\exp(U/kT)}{x^2} dx]^{-1}$$

(general case, taking into account interaction potential)

Hydrated electron:

$k_{dif} \sim 10^{10}\ M^{-1}c^{-1}$

R ~ 0.25 нм

Reaction kinetics of e^-_{aq}: other cases

- 2. Slow reactions : $k \ll k_{dif}$

$$e^-_{aq} + C_6H_6 \rightarrow C_6H_6^{-\cdot} \quad (k = 1.2 \cdot 10^7\ M^{-1}c^{-1})$$

$$e^-_{aq} + CH_3OH \rightarrow CH_3O^- + H^\cdot \quad (k < 10^4\ M^{-1}c^{-1})$$

Complex multi-step mechanisms

- 3. Ultrafast reactions: $k > k_{dif}$

$$e^-_{aq} + CHCl_3 \rightarrow CHCl_2 + Cl^- \ (k = 3 \cdot 10^{10}\ M^{-1}c^{-1})$$

Formal “reaction radius” $r > R_A + R_B$ (up to 1 – 1.5 нм) →distant transfer (contribution of tuneling)

(novel interpretation may come from recent MD findings)

Applications of slolvated electron: inorgaic chemistry and technology

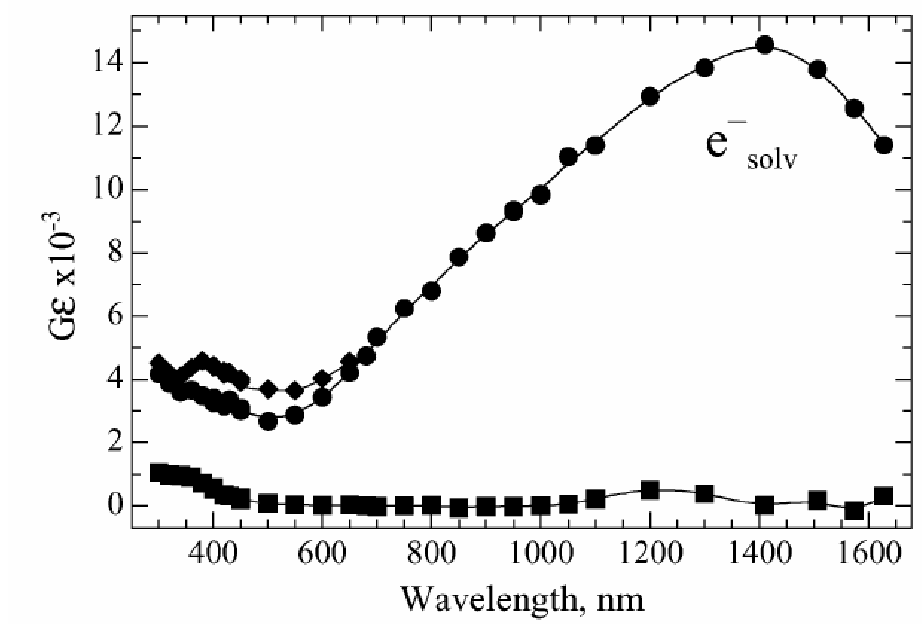
- Elucidation of the mechanisms of inorganic reactions with electron transfer
- Studies on metal ions in unusual oxidation states: *Cd(I), Zn(I), Hg(I), In (II), Eu (II), Yb (II), Sm (II), Am (II), etc.*
- Obtaining spectral properties of neutral atoms in solutions (e.g., Pb^0 , Ag^0)
- Structure and reaction kinetics of inorganic radicals
- Preparation of metal clusters and nanoparticles by ion reduction (especially, from non-noble metals)
- Purification of waste water

Application of solvated electron: organic chemistry and biochemistry

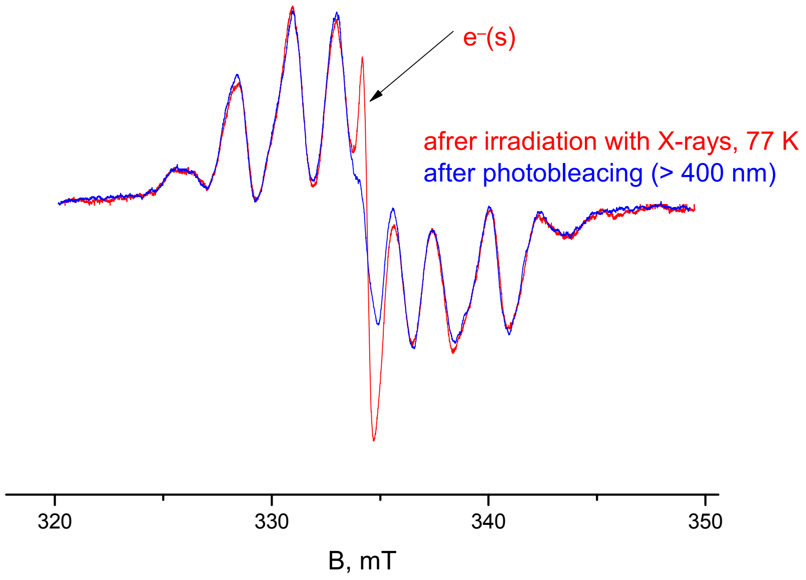
- Mechanisms of organic electron-transfer reactions
- Direct characterization of unstable organic radicals and radical anions in solutions
- Selective preparative reduction of organic compounds
- Modeling electron transfer in biology, in particular in organized systems (photosynthesis, enzymatic reactions, etc.)
- Investigation of non-oxidative radiation damage of biomolecules, mecanisms of radioprotective and antioxidative activity

Excess electron in ionic liquids

- What happens to an excess electron injected to an IL:
  - (i) going to cation to yield radical?
  - (ii) going to anion to yield dianion ?
  - (iii) creates a “cavity” ?



First indication of optical spectrum
of “solvated electron in R4NNTf2
(*Wishart & Neta, JPC B, 2003, 107, 7261*)



An EPR evidence for a “cavity-like” species in
1-butyl-1-methyl pyrrolidinium bis(trifluoromethane
sulfonyl)imide (P_{14})
(Saenko, Takahasi & Feldman, 2012)

Conclusions....

- **Solvated electron is**
- **a well-documented and extensively studied species,**
- an useful concept for differnet fields of condensed-phase chemistry and chemical physics
- coming to technology

- **However...**
- **We still do not understand completely, what is it...**

...and outlook

- **Challenges:**
- - ultrafast dynamics of electron solvation
- - solvated electrons in novel media (IL, supercritical water, etc.)
- - electron solvation in confined media (nanopores), surfaces and interfaces (structural and dynamic aspects)
- - rigorous theoretical treatment of kinetics in view of recent MD findings
- - development of “electron solvation probing”
- - biological implications

- **→...development of a compehensive realistic model**