Холодные ~~нейтроны~~ молекулы: получение и спектроскопия

Исаев Т.А.

ПИЯФ НИЦ КИ, ОНИ

14 October, 2015

Холодная материя

<table>
<tr><td>(Ультра)Холодные нейтроны</td><td>(Ультра)Холодные атомы /молекулы</td></tr>
<tr><td colspan="2">~ 1 K
Прецизионные измерения (длительное время хранения, контролируемые внешние поля)</td></tr>
<tr><td>Слабо взаимодействуют с электромагнитными полями
Получение и контроль при взаимодействии с холодным веществом или сильными магнитами полями
Трудно наблюдать коллективные (многочастичные) состояния</td><td>Сильное взаимодействие со светом и внешними электромагнитными полями
Наиболее эффективный метод получения холодных атомов - лазерное охлаждение
Хорошо взаимодействуют за счет магнитного (μ_B) и электрического (D) моментов</td></tr>
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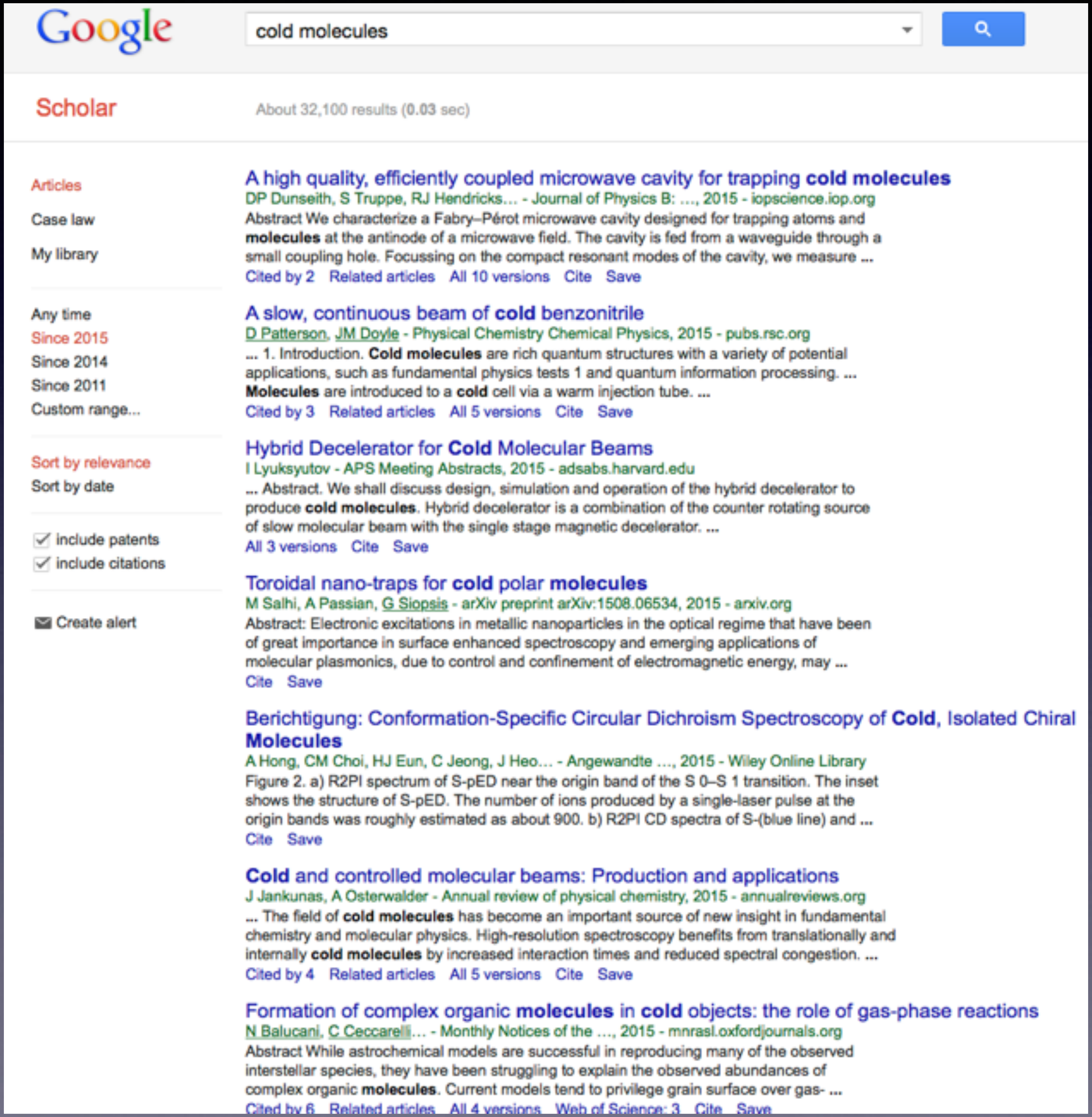
Холодные молекулы: зачем?



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A high quality, efficiently coupled microwave cavity for trapping **cold molecules**
DP Dunseith, S Truppe, RJ Hendricks... - Journal of Physics B: ..., 2015 - iopscience.iop.org
Abstract We characterize a Fabry–Pérot microwave cavity designed for trapping atoms and **molecules** at the antinode of a microwave field. The cavity is fed from a waveguide through a small coupling hole. Focussing on the compact resonant modes of the cavity, we measure ...
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A slow, continuous beam of **cold** benzonitrile
D Patterson, JM Doyle - Physical Chemistry Chemical Physics, 2015 - pubs.rsc.org
... 1. Introduction. **Cold molecules** are rich quantum structures with a variety of potential applications, such as fundamental physics tests 1 and quantum information processing. ... **Molecules** are introduced to a **cold** cell via a warm injection tube. ...
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Hybrid Decelerator for **Cold** Molecular Beams
I Lyuksyutov - APS Meeting Abstracts, 2015 - adsabs.harvard.edu
... Abstract. We shall discuss design, simulation and operation of the hybrid decelerator to produce **cold molecules**. Hybrid decelerator is a combination of the counter rotating source of slow molecular beam with the single stage magnetic decelerator. ...
All 3 versions Cite Save

Toroidal nano-traps for **cold** polar **molecules**
M Salhi, A Passian, G Siopsis - arXiv preprint arXiv:1508.06534, 2015 - arxiv.org
Abstract: Electronic excitations in metallic nanoparticles in the optical regime that have been of great importance in surface enhanced spectroscopy and emerging applications of molecular plasmonics, due to control and confinement of electromagnetic energy, may ...
Cite Save

Berichtigung: Conformation-Specific Circular Dichroism Spectroscopy of **Cold**, Isolated Chiral **Molecules**
A Hong, CM Choi, HJ Eun, C Jeong, J Heo... - Angewandte ..., 2015 - Wiley Online Library
Figure 2. a) R2PI spectrum of S-pED near the origin band of the S 0–S 1 transition. The inset shows the structure of S-pED. The number of ions produced by a single-laser pulse at the origin bands was roughly estimated as about 900. b) R2PI CD spectra of S-(blue line) and ...
Cite Save

Cold and controlled molecular beams: Production and applications
J Jankunas, A Osterwalder - Annual review of physical chemistry, 2015 - annualreviews.org
... The field of **cold molecules** has become an important source of new insight in fundamental chemistry and molecular physics. High-resolution spectroscopy benefits from translationally and internally **cold molecules** by increased interaction times and reduced spectral congestion. ...
Cited by 4 Related articles All 5 versions Cite Save

Formation of complex organic **molecules** in **cold** objects: the role of gas-phase reactions
N Balucani, C Ceccarelli... - Monthly Notices of the ..., 2015 - mnrasl.oxfordjournals.org
Abstract While astrochemical models are successful in reproducing many of the observed interstellar species, they have been struggling to explain the observed abundances of complex organic **molecules**. Current models tend to privilege grain surface over gas- ...
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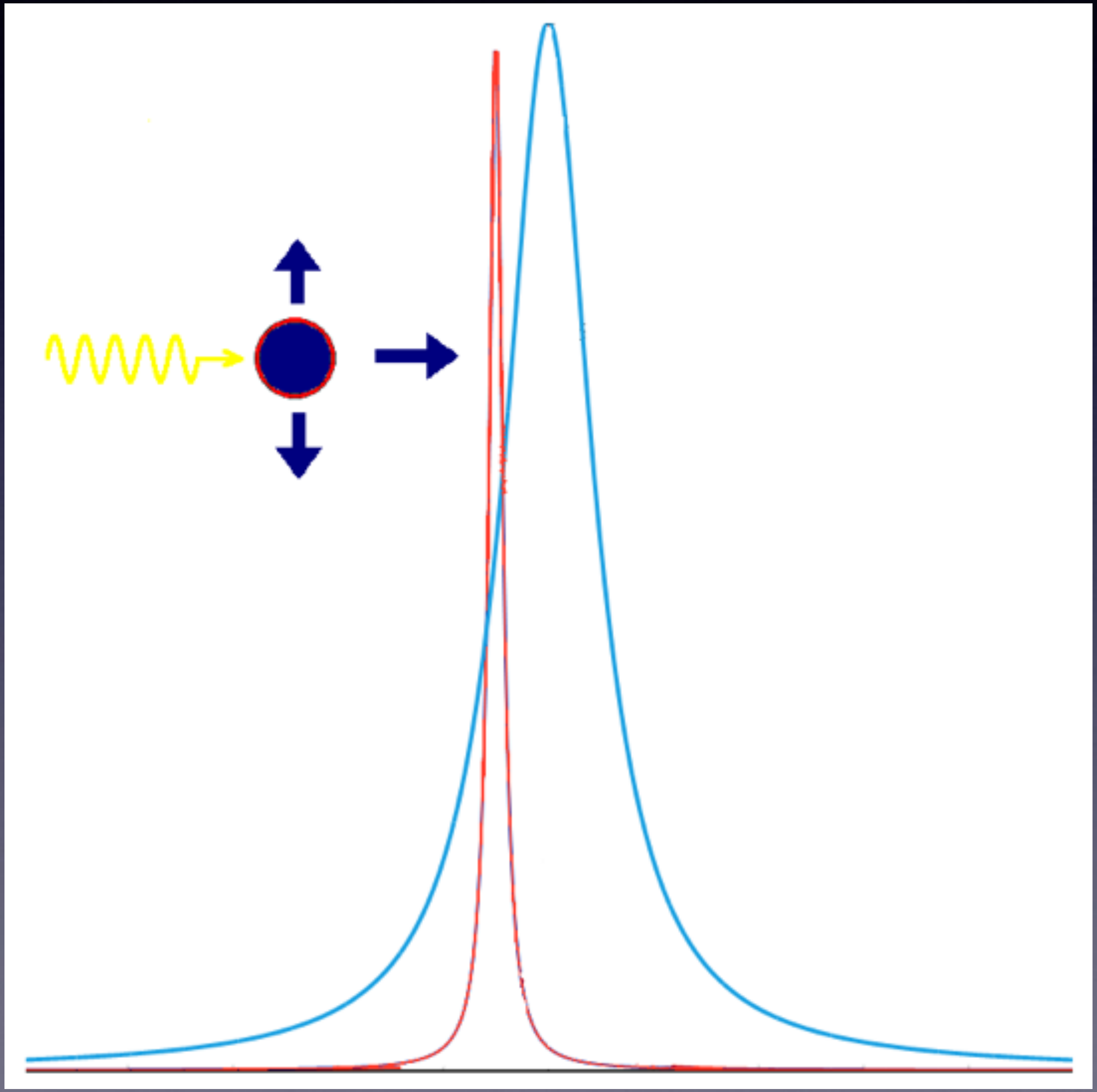
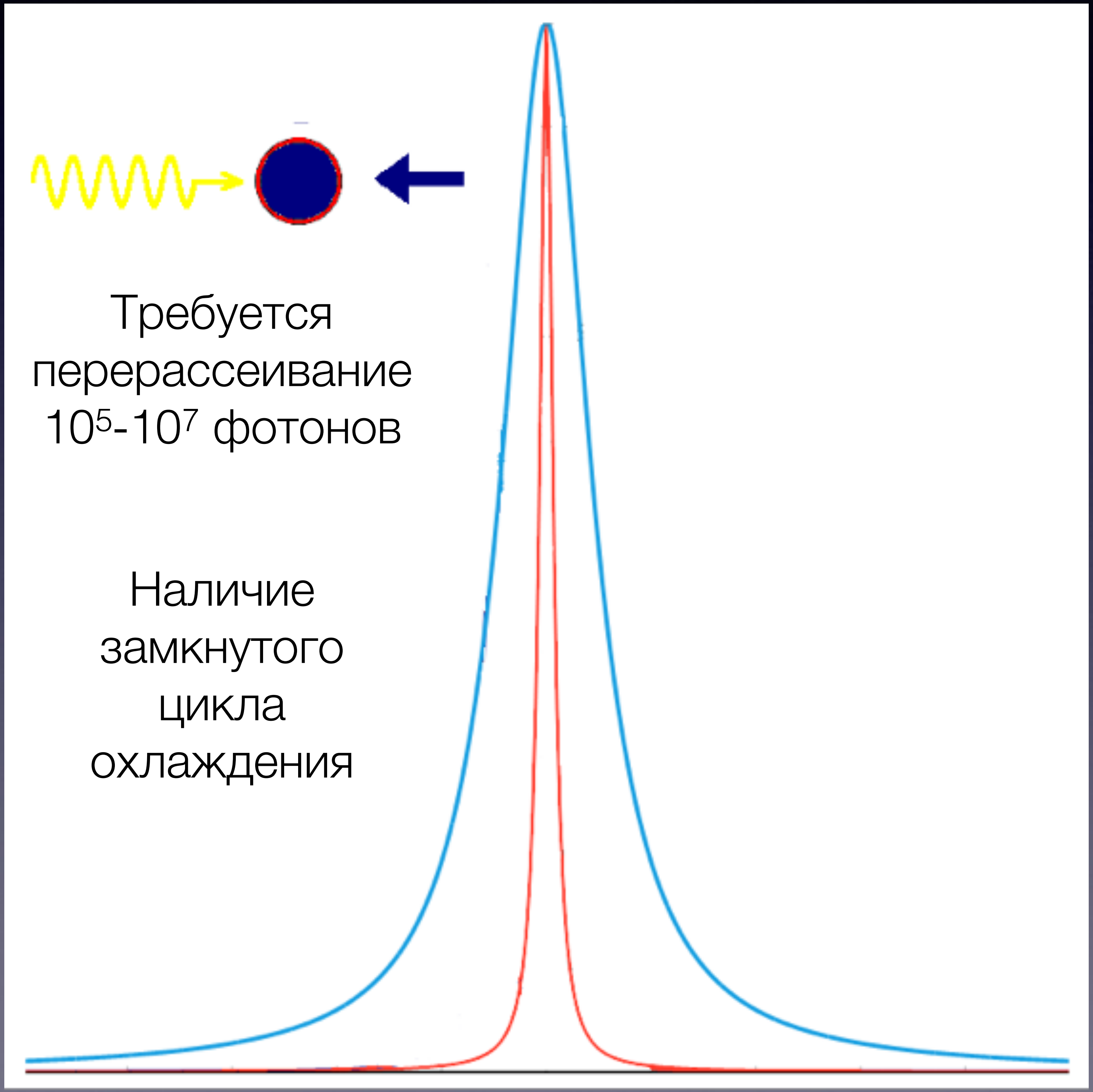
Лазерное (допплеровское) торможение, охлаждение и хранение.



Лазерное (допплеровское) торможение, охлаждение и хранение.



Требуется перерассеивание 10^5-10^7 фотонов

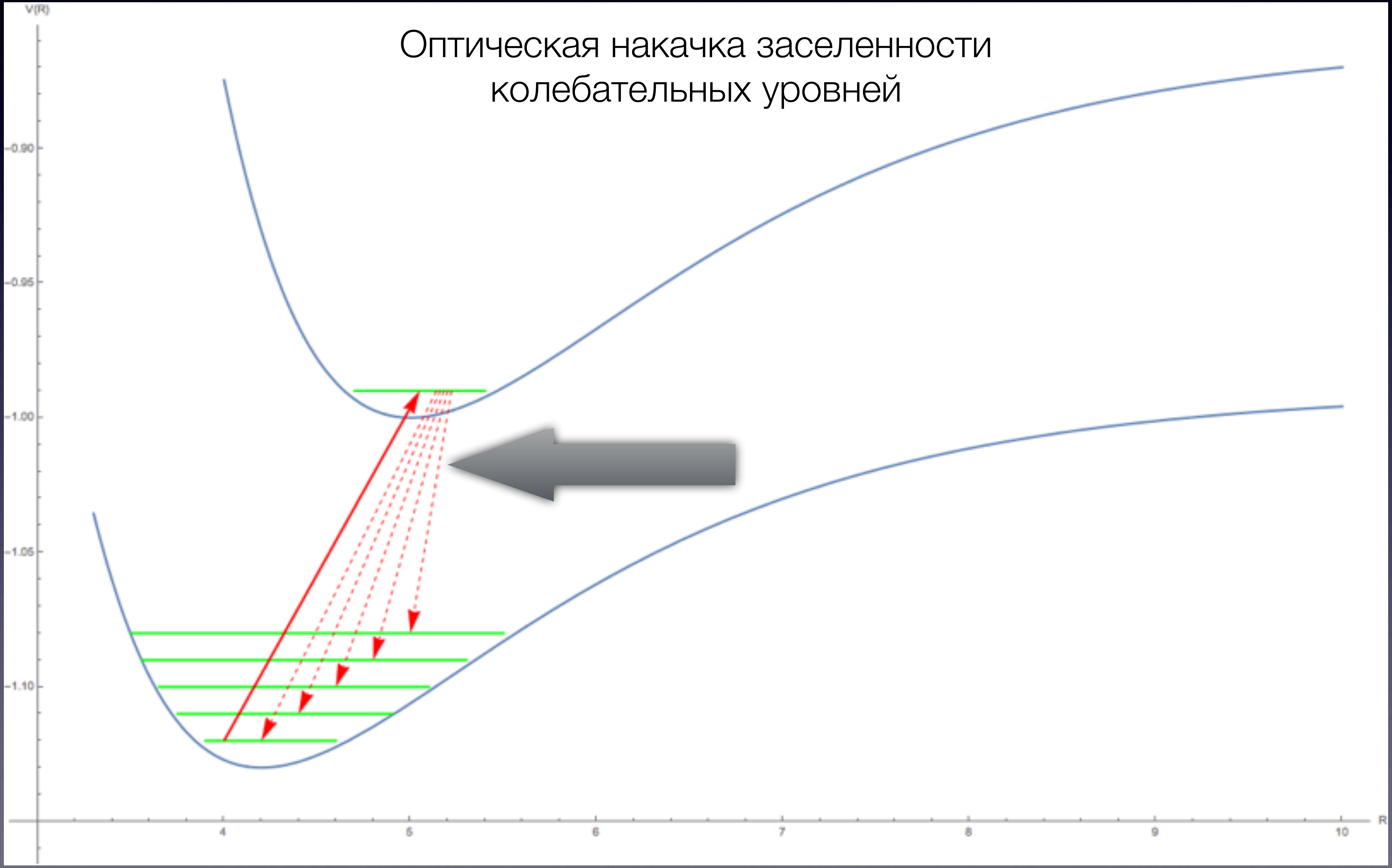
Наличие замкнутого цикла охлаждения

Холодные молекулы

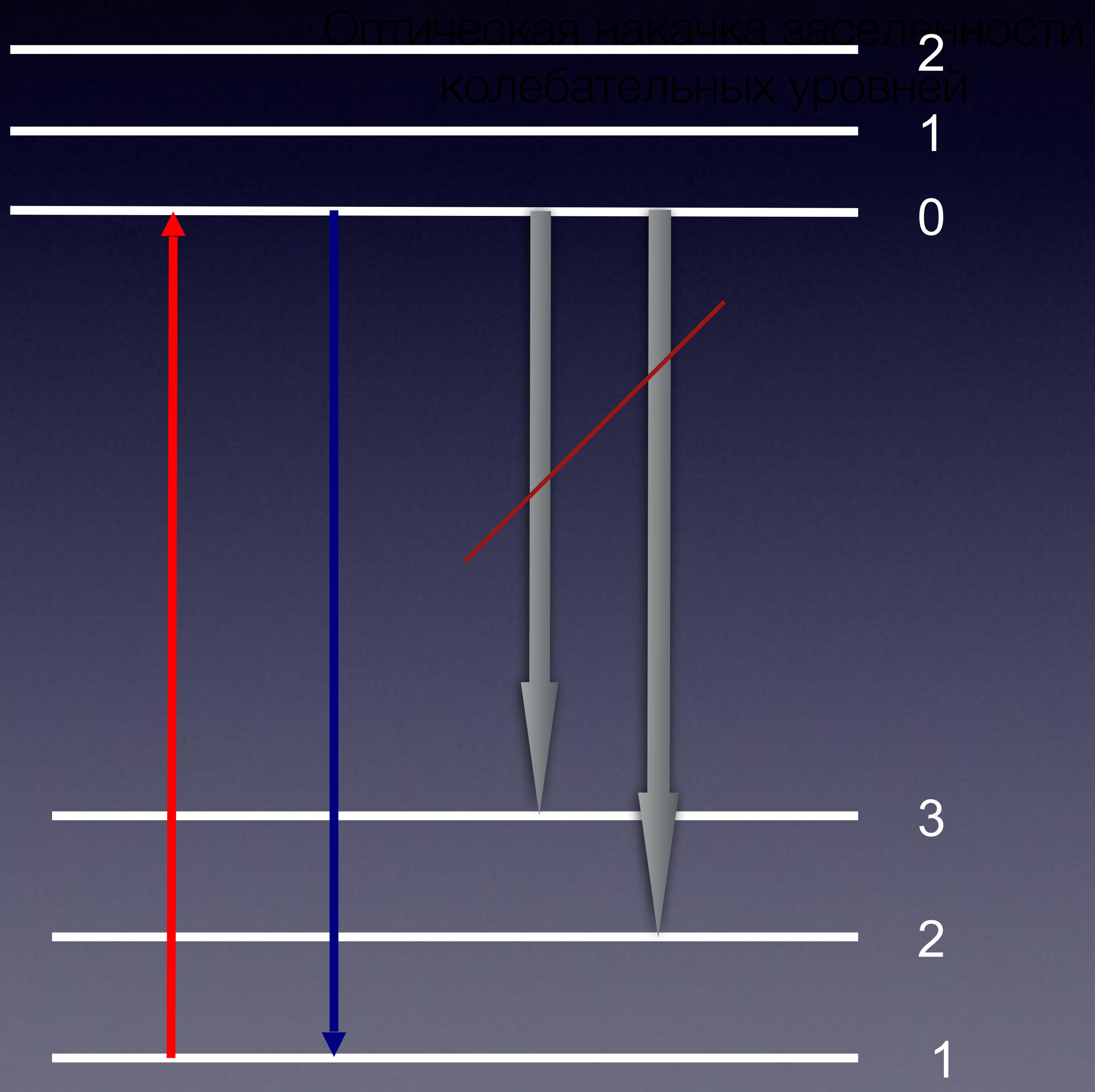
Таблица из статьи M. Schnell and G. Meijer, Angew. Chem. Int. Ed. ***48****, 6010 (2009)*

Method	Molecules	T	N
Photoassociation	Rb_2, Cs_2, He_2, H_2, Li_2, Na_2, K_2, Ca_2, KRb, RbCs, NaCs, LiCs, LiRb	30 μK	10^5
Feshbach/STIRAP	Li_2, Na_2, K_2, Rb_2, Cs_2, KRb	50 *n*K	$>10^5$
Buffer-gas cooling	CaH, CaF, VO, PbO, NH, CrH, MnH	400 *m*K	$>10^8$
Stark deceleration/ Trapping	NH_3, CO, OH, NH, SO_2, YbF, H_2CO, C_7H_5N	5 *m*K	10^6
Doppler cooling	??????????????????????		

Холодные молекулы


Оптическая накачка заселенности
колебательных уровней

Правила отбора по вращательному квантовому числу



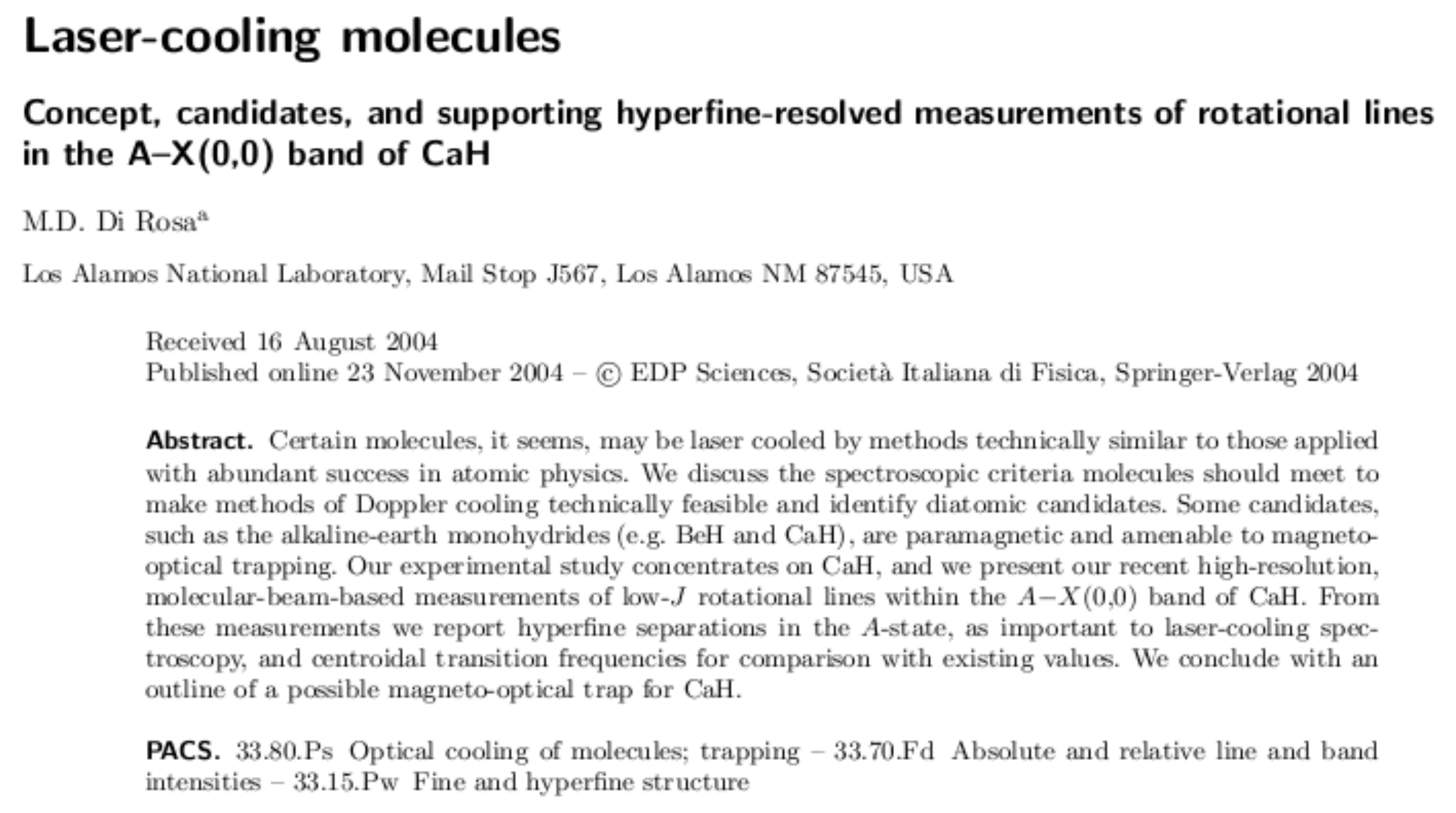
Электрический дипольный переход между электронными уровнями в двухатомной молекуле

Оптическая накачка заселенности колебательных уровней

$$\boldsymbol{\mu}_e(f, i) = \langle J, M|\cos\theta|J', M'\rangle \boxed{\left[\int_\alpha \psi_v^*(R_\alpha)\psi_v'(R_\alpha)\,\mathrm{d}V_\alpha\right]} \times \left[-e\int_i \psi_e^*(r_i, R_\alpha)\sum_i \boldsymbol{r}_i\psi_e'(r_i, R_\alpha)\,\mathrm{d}V_i\right],$$

Прямое (допплеровское) лазерное охлаждение

Оптическая накачка заселенности



Laser-cooling molecules

Concept, candidates, and supporting hyperfine-resolved measurements of rotational lines in the A–X(0,0) band of CaH

M.D. Di Rosa[a]

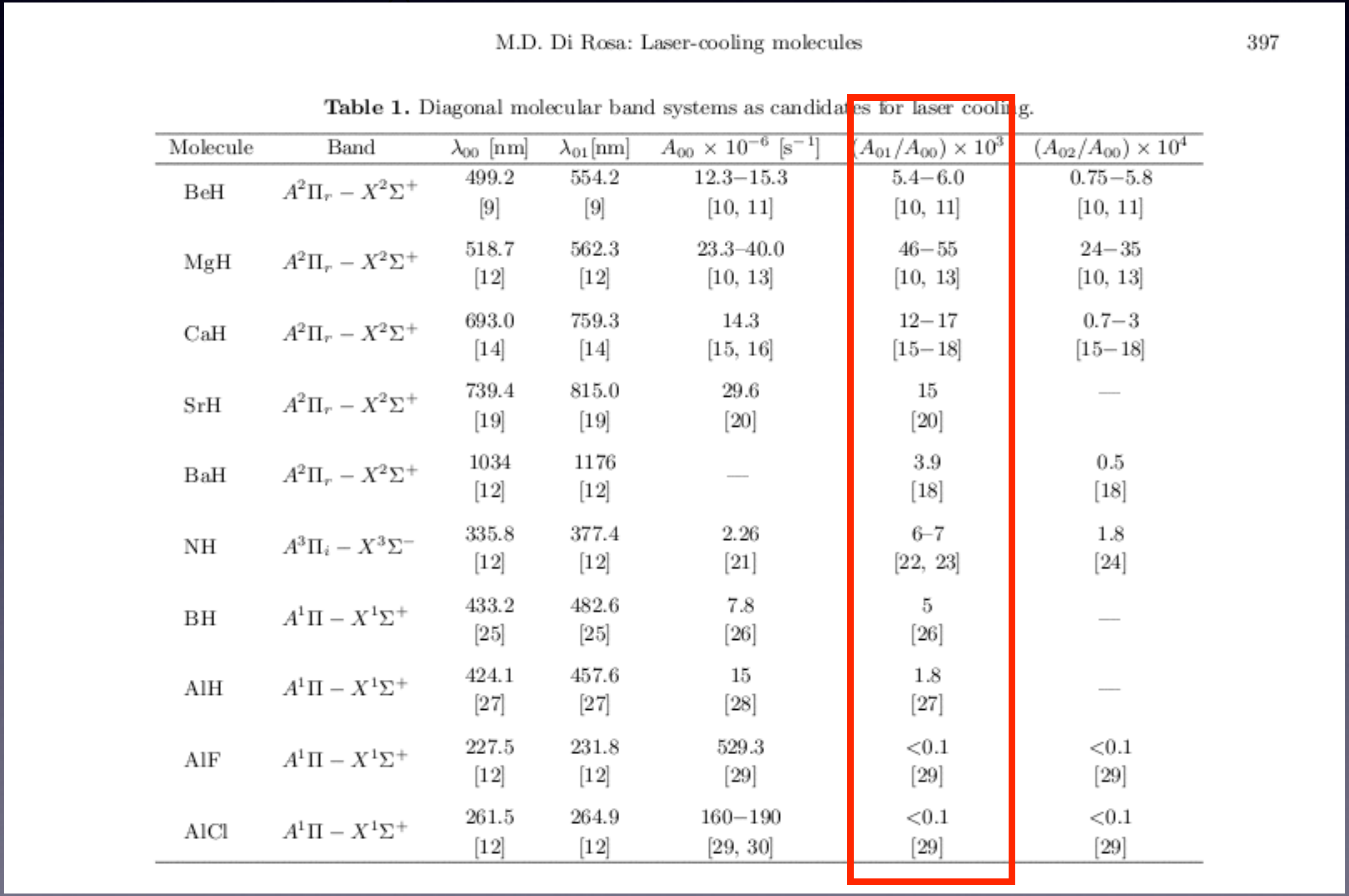
Los Alamos National Laboratory, Mail Stop J567, Los Alamos NM 87545, USA

Received 16 August 2004

Abstract. Certain molecules, it seems, may be laser cooled by methods technically similar to those applied with abundant success in atomic physics. We discuss the spectroscopic criteria molecules should meet to make methods of Doppler cooling technically feasible and identify diatomic candidates. Some candidates, such as the alkaline-earth monohydrides (e.g. BeH and CaH), are paramagnetic and amenable to magneto-optical trapping. Our experimental study concentrates on CaH, and we present our recent high-resolution, molecular-beam-based measurements of low-J rotational lines within the $A{-}X(0,0)$ band of CaH. From these measurements we report hyperfine separations in the A-state, as important to laser-cooling spectroscopy, and centroidal transition frequencies for comparison with existing values. We conclude with an outline of a possible magneto-optical trap for CaH.

PACS. 33.80.Ps Optical cooling of molecules; trapping – 33.70.Fd Absolute and relative line and band intensities – 33.15.Pw Fine and hyperfine structure

Прямое (допплеровское) лазерное охлаждение



M.D. Di Rosa: Laser-cooling molecules 397

Table 1. Diagonal molecular band systems as candidates for laser cooling.

Molecule	Band	λ_{00} [nm]	λ_{01}[nm]	$A_{00} \times 10^{-6}$ [s^{-1}]	$(A_{01}/A_{00}) \times 10^3$	$(A_{02}/A_{00}) \times 10^4$
BeH	$A^2\Pi_r - X^2\Sigma^+$	499.2 [9]	554.2 [9]	12.3–15.3 [10, 11]	5.4–6.0 [10, 11]	0.75–5.8 [10, 11]
MgH	$A^2\Pi_r - X^2\Sigma^+$	518.7 [12]	562.3 [12]	23.3–40.0 [10, 13]	46–55 [10, 13]	24–35 [10, 13]
CaH	$A^2\Pi_r - X^2\Sigma^+$	693.0 [14]	759.3 [14]	14.3 [15, 16]	12–17 [15–18]	0.7–3 [15–18]
SrH	$A^2\Pi_r - X^2\Sigma^+$	739.4 [19]	815.0 [19]	29.6 [20]	15 [20]	—
BaH	$A^2\Pi_r - X^2\Sigma^+$	1034 [12]	1176 [12]	—	3.9 [18]	0.5 [18]
NH	$A^3\Pi_i - X^3\Sigma^-$	335.8 [12]	377.4 [12]	2.26 [21]	6–7 [22, 23]	1.8 [24]
BH	$A^1\Pi - X^1\Sigma^+$	433.2 [25]	482.6 [25]	7.8 [26]	5 [26]	—
AlH	$A^1\Pi - X^1\Sigma^+$	424.1 [27]	457.6 [27]	15 [28]	1.8 [27]	—
AlF	$A^1\Pi - X^1\Sigma^+$	227.5 [12]	231.8 [12]	529.3 [29]	<0.1 [29]	<0.1 [29]
AlCl	$A^1\Pi - X^1\Sigma^+$	261.5 [12]	264.9 [12]	160–190 [29, 30]	<0.1 [29]	<0.1 [29]

О замкнутости охлаждающего цикла

Число фотонов ФК - фактор	1000	10000	100000	1000000
0.90000	0	0	0	0
0.99000	0.0000431	0	0	0
0.99900	0.367695	0.0000451	0	0
0.99990	0.904833	0.367861	0.0000453	0
0.99999	0.99005	0.904837	0.367878	0.0000453

О замкнутости охлаждающего цикла

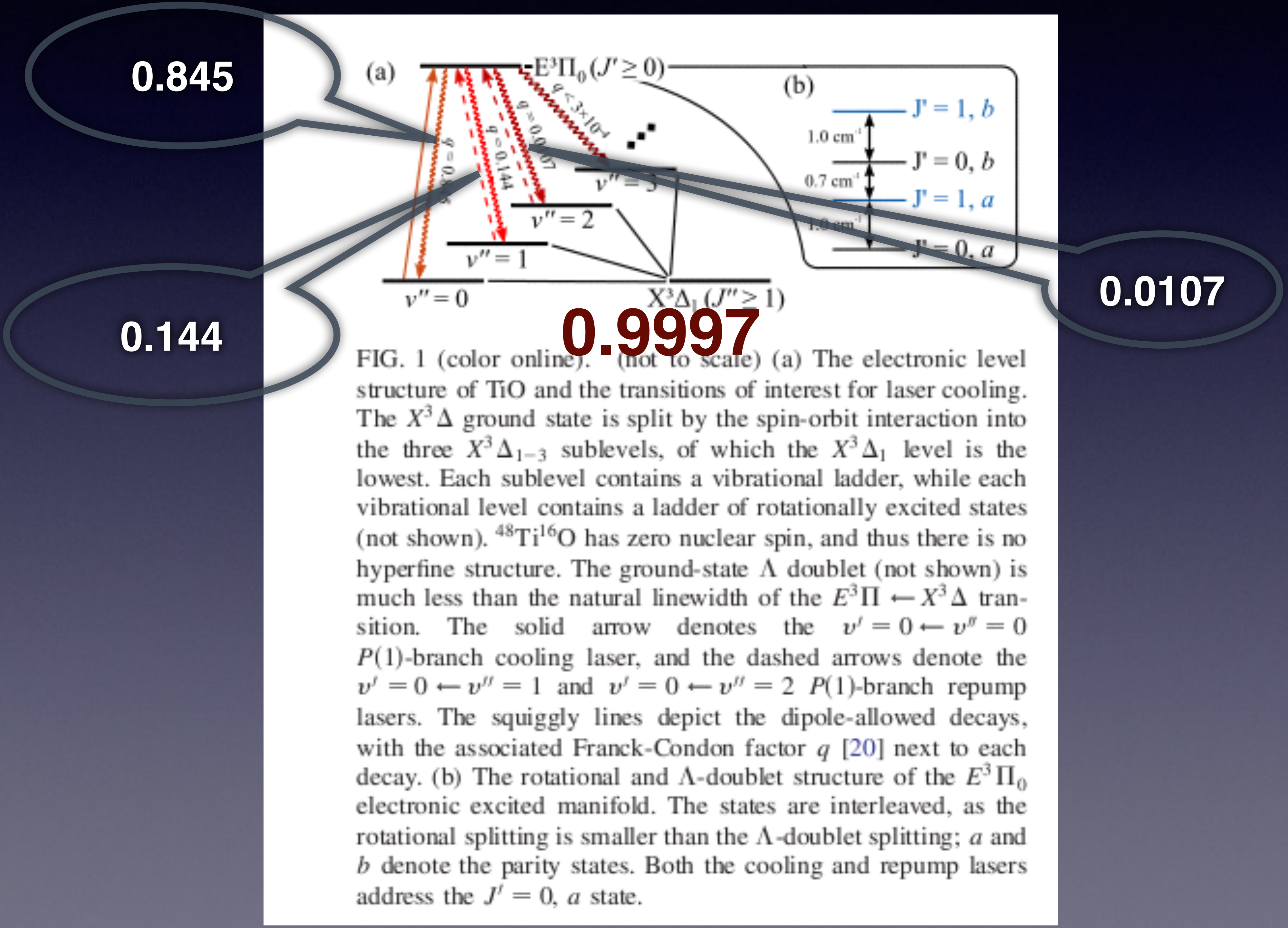


FIG. 1 (color online). (not to scale) (a) The electronic level structure of TiO and the transitions of interest for laser cooling. The $X^3\Delta$ ground state is split by the spin-orbit interaction into the three $X^3\Delta_{1-3}$ sublevels, of which the $X^3\Delta_1$ level is the lowest. Each sublevel contains a vibrational ladder, while each vibrational level contains a ladder of rotationally excited states (not shown). ^{48}Ti^{16}O has zero nuclear spin, and thus there is no hyperfine structure. The ground-state Λ doublet (not shown) is much less than the natural linewidth of the $E^3\Pi \leftarrow X^3\Delta$ transition. The solid arrow denotes the $v' = 0 \leftarrow v'' = 0$ $P(1)$-branch cooling laser, and the dashed arrows denote the $v' = 0 \leftarrow v'' = 1$ and $v' = 0 \leftarrow v'' = 2$ $P(1)$-branch repump lasers. The squiggly lines depict the dipole-allowed decays, with the associated Franck-Condon factor q [20] next to each decay. (b) The rotational and Λ-doublet structure of the $E^3\Pi_0$ electronic excited manifold. The states are interleaved, as the rotational splitting is smaller than the Λ-doublet splitting; a and b denote the parity states. Both the cooling and repump lasers address the $J' = 0$, a state.
]

Когда возникает диагональная франк-кондоновская матрица

Оптическая накачка заселенности колебательных уровней

- Одинаковая форма (параллельность) потенциальных кривых
- Тогда колебательные волновые функции отличаются только фазой (энергией)
- ФК матрица практически диагональна

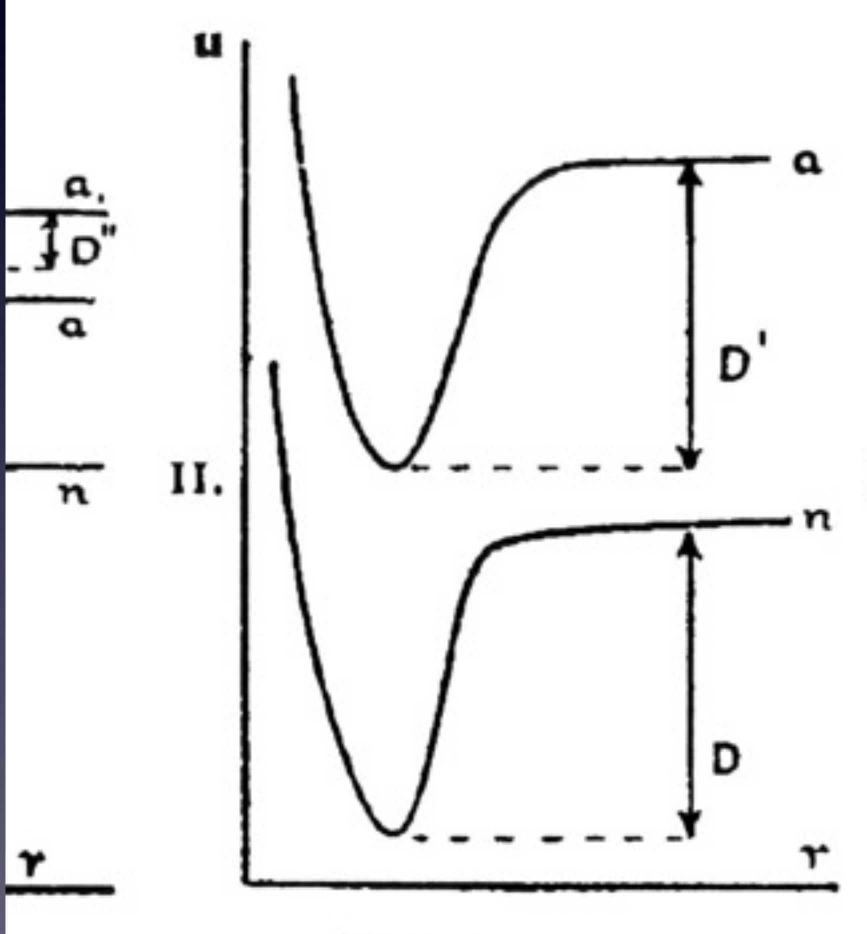
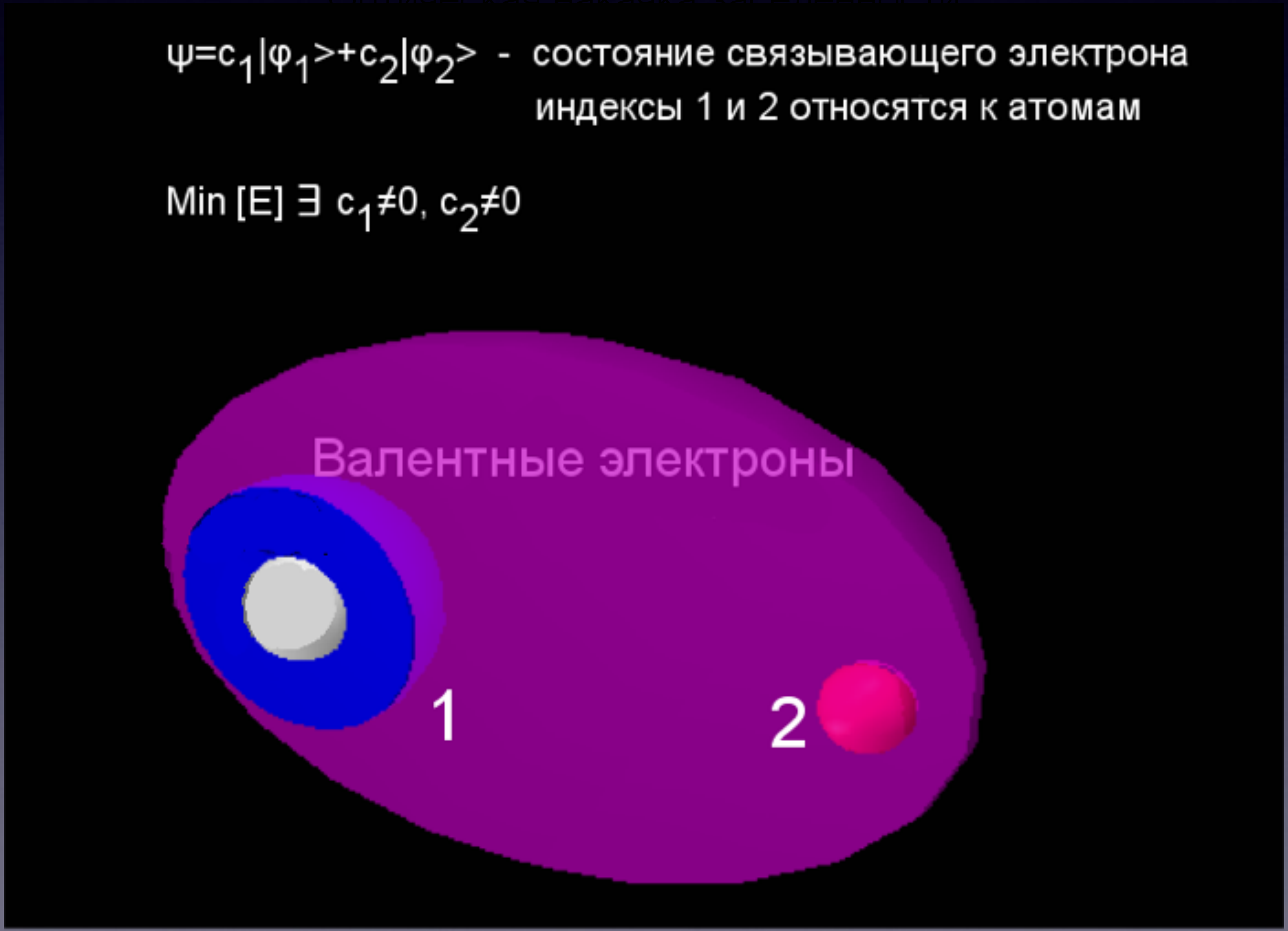


Fig. I.

Химическая связь в двухатомных молекулах

Оптическая накачка заселенности



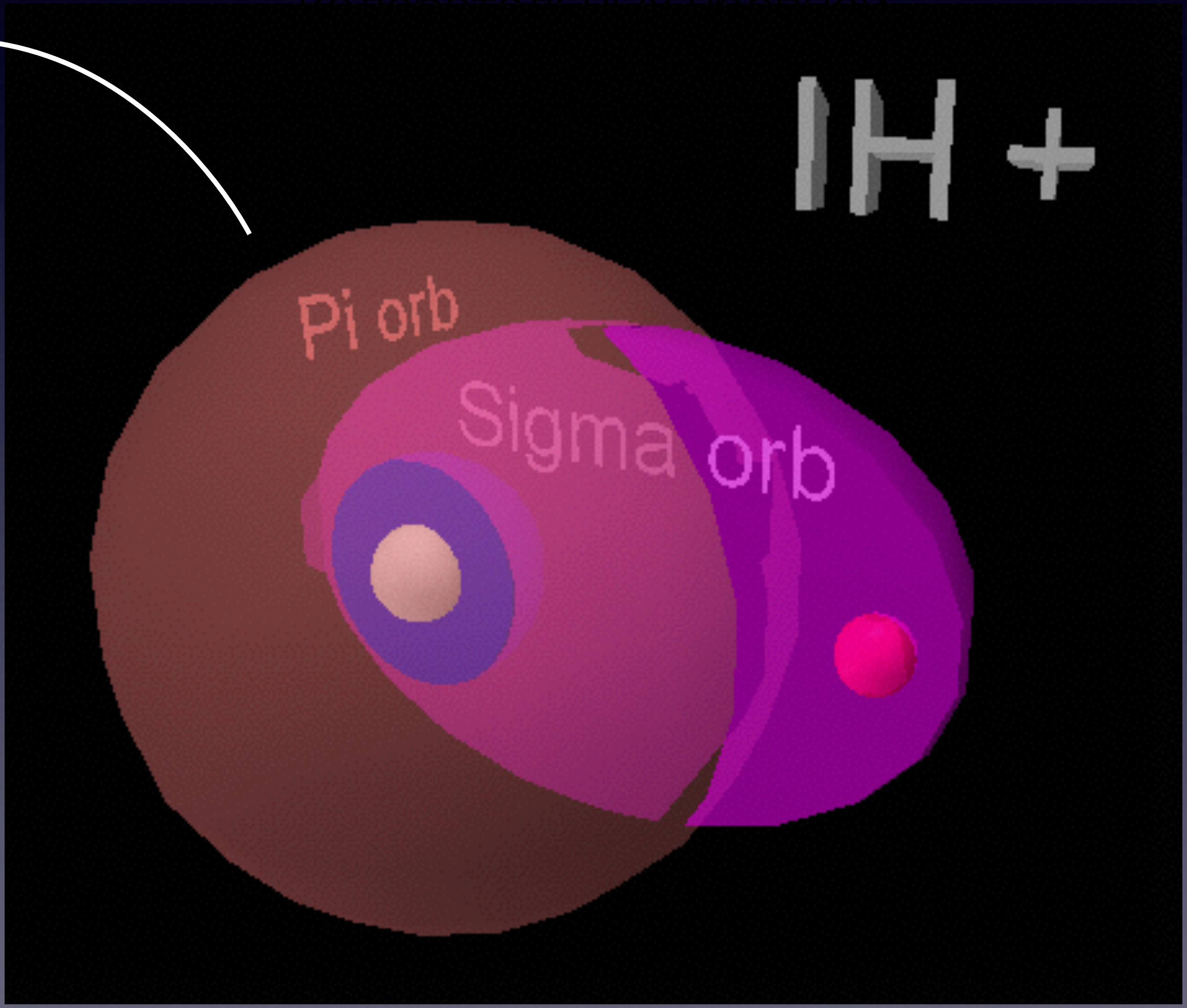
$\psi = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$ - состояние связывающего электрона
индексы 1 и 2 относятся к атомам

Min [E] $\exists$ $c_1 \neq 0$, $c_2 \neq 0$

Химическая связь в двухатомных молекулах

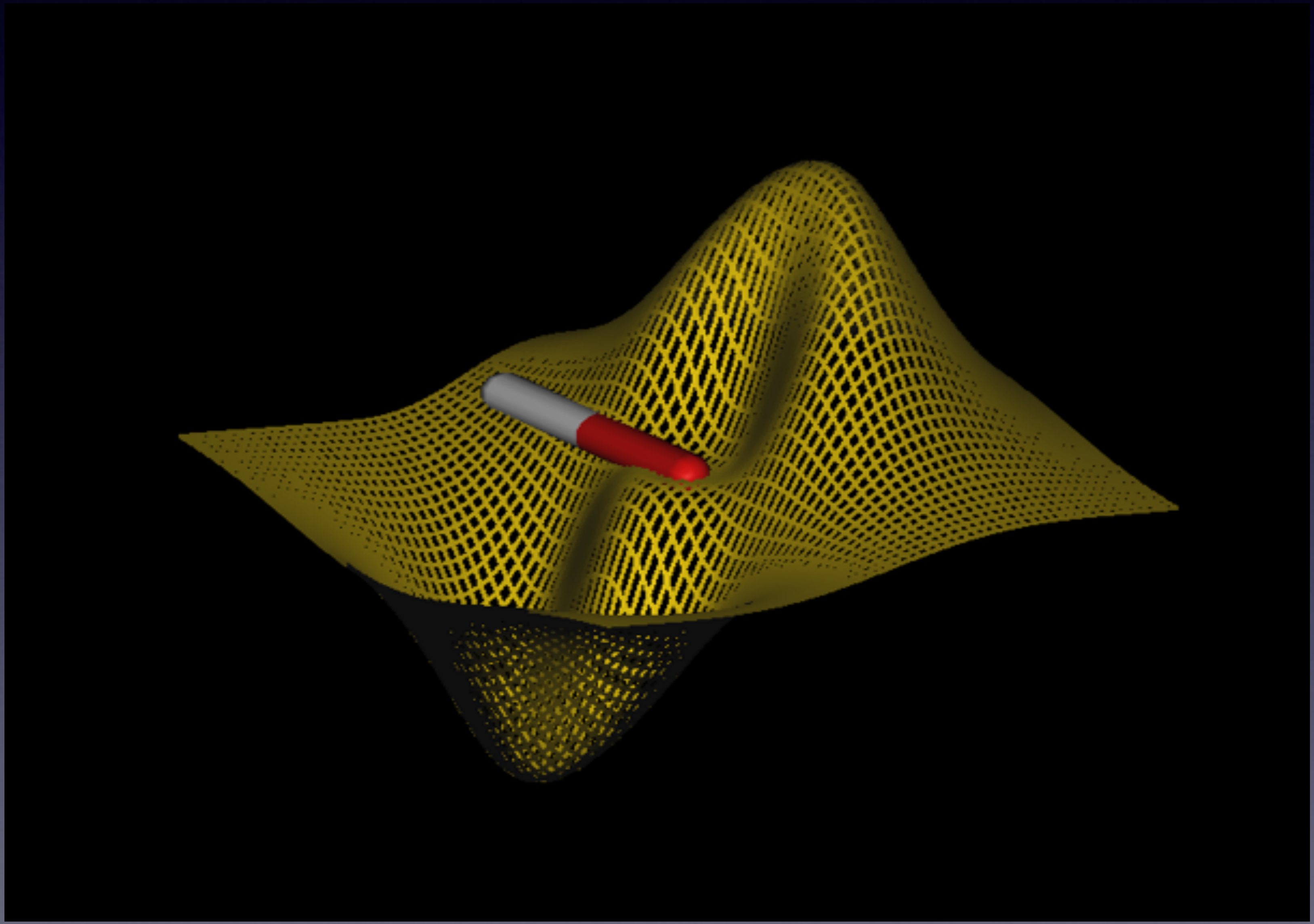
Оптическая накачка заселенности

П$_{3/2}$

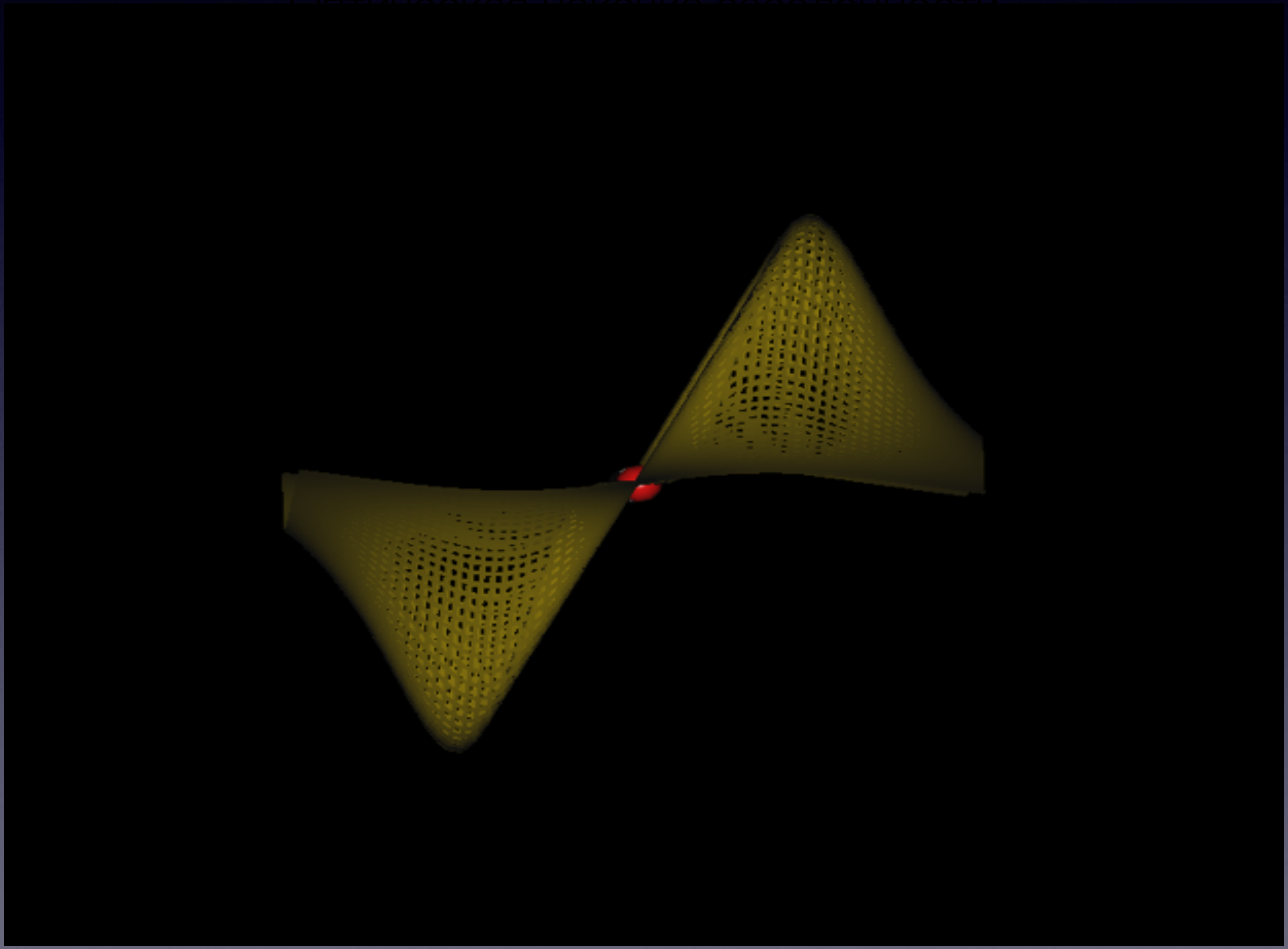


Химическая связь в двухатомных молекулах

Оптическая накачка заселенности

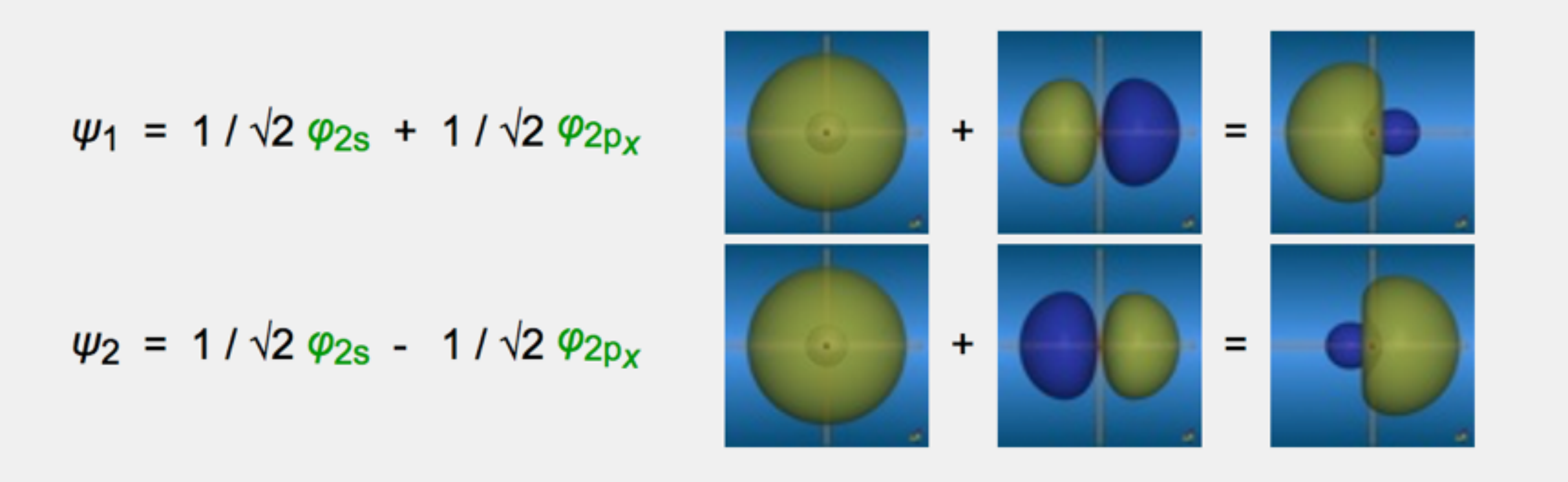


Химическая связь в двухатомных молекулах



Химическая связь в двухатомных молекулах

Оптическая накачка заселенности колебательных уровней



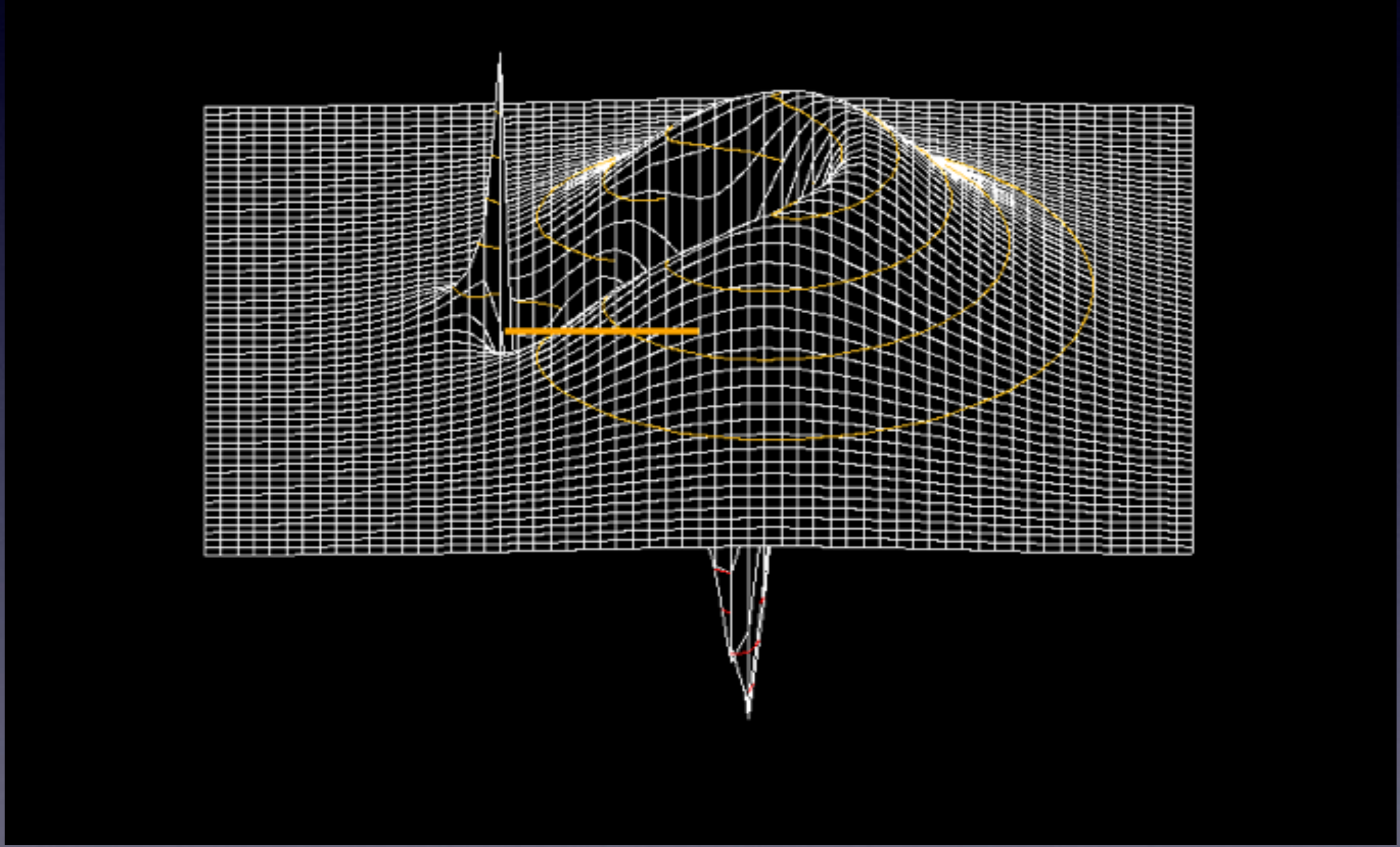
$$\psi_1 = 1/\sqrt{2}\,\varphi_{2s} + 1/\sqrt{2}\,\varphi_{2p_x}$$

$$\psi_2 = 1/\sqrt{2}\,\varphi_{2s} - 1/\sqrt{2}\,\varphi_{2p_x}$$

Химическая связь в двухатомных молекулах

Оптическая накачка заселенности

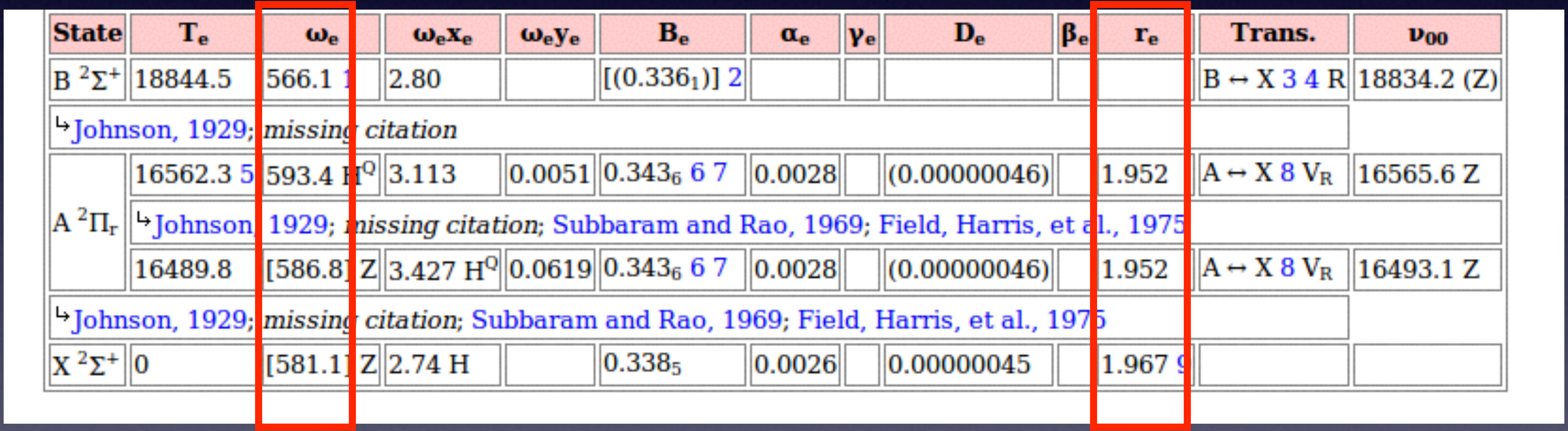
CaF



Химическая связь в двухатомных молекулах

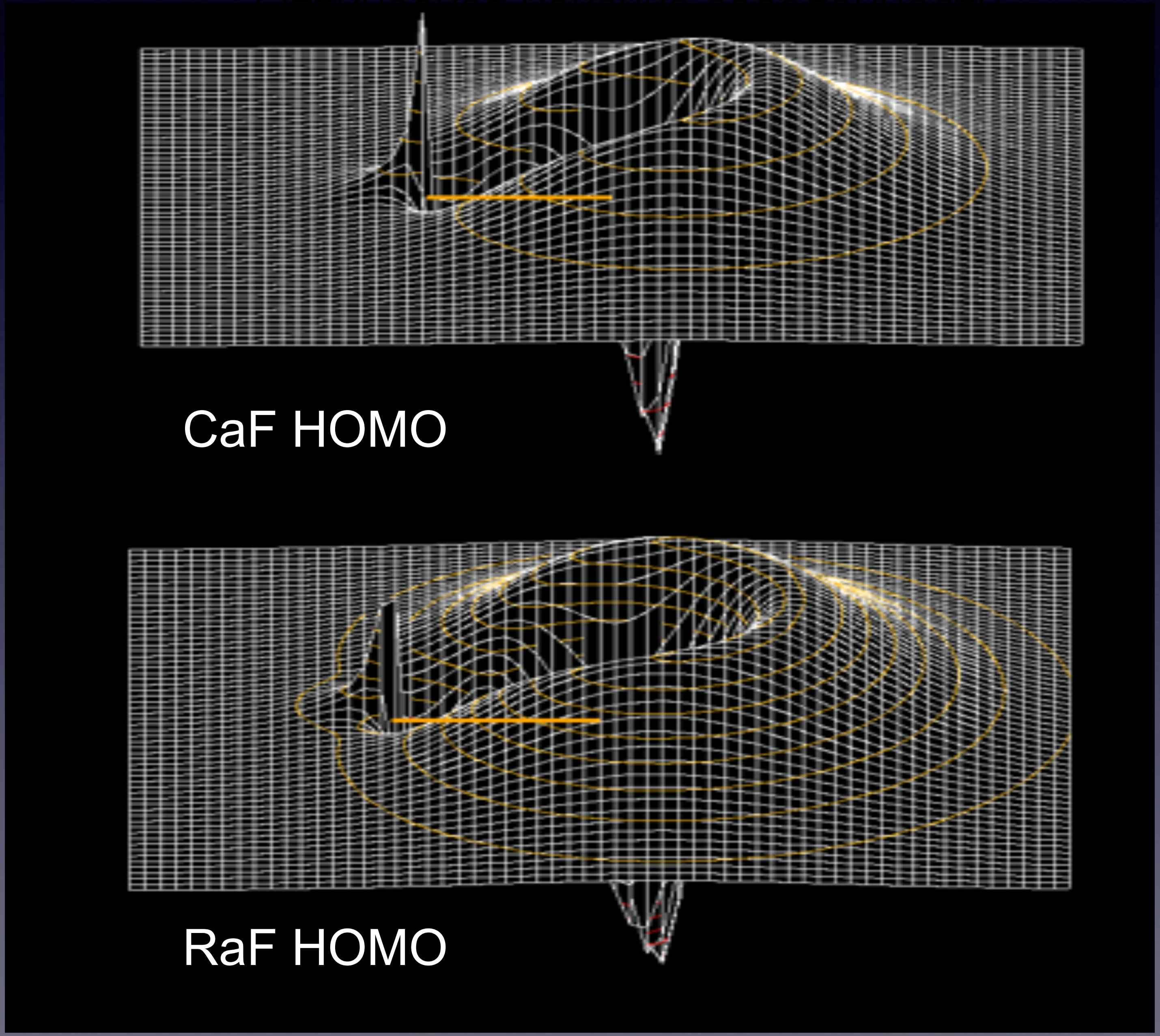
CaF

Оптическая накачка заселенности колебательных уровней



State	T_e	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	γ_e	D_e	β_e	r_e	Trans.	ν_{00}
B $^2\Sigma^+$	18844.5	566.1 1	2.80		[(0.336$_1$)] 2						B ↔ X 3 4 R	18834.2 (Z)
↳Johnson, 1929; *missing citation*												
A $^2\Pi_r$	16562.3 5	593.4 H^Q	3.113	0.0051	0.343$_6$ 6 7	0.0028		(0.00000046)		1.952	A ↔ X 8 V$_R$	16565.6 Z
	↳Johnson, 1929; *missing citation*; Subbaram and Rao, 1969; Field, Harris, et al., 1975											
	16489.8	[586.8] Z	3.427 H^Q	0.0619	0.343$_6$ 6 7	0.0028		(0.00000046)		1.952	A ↔ X 8 V$_R$	16493.1 Z
↳Johnson, 1929; *missing citation*; Subbaram and Rao, 1969; Field, Harris, et al., 1975												
X $^2\Sigma^+$	0	[581.1] Z	2.74 H		0.338$_5$	0.0026		0.00000045		1.967 9		

Химическая связь в двухатомных молекулах



Предложение по кандидатам для охлаждения

Соединение с несвязывающей орбиталью первого типа - RaF

Соединение с несвязывающей орбиталью второго типа - PoH

Соединения переходных металлов

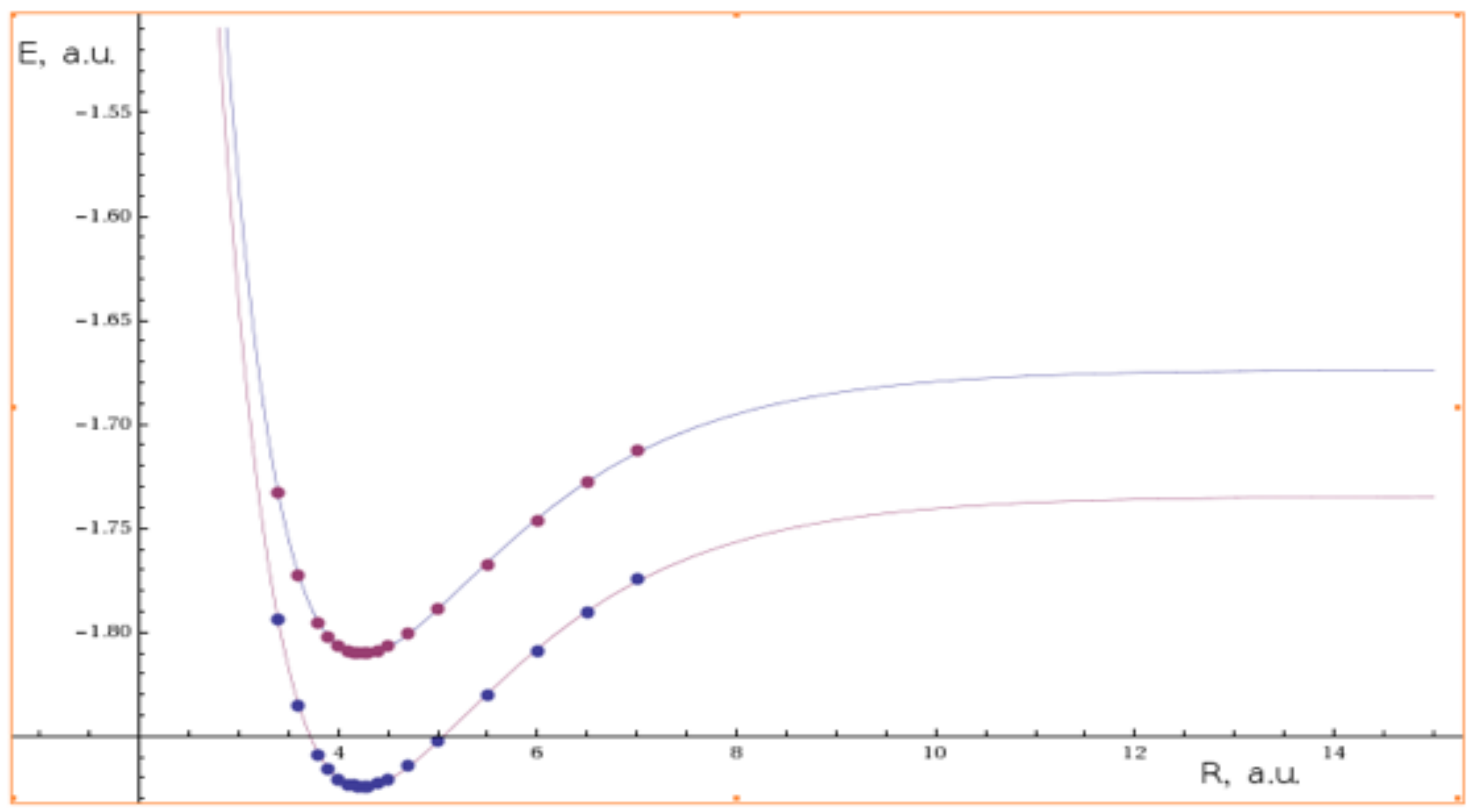
** Previous IUPAC numbering system

*** Numbering system recommended by the Chemical Abstracts Service

**** For the names of elements 104–112, see Table 27.

RaF

	Re, a.u.	β
$^2\Sigma$	4.24377	0.666022
$^2\Pi$	4.23951	0.666897



RaF

- Очень перспективный кандидат для поиска “новой физики” (уже идут измерения на атомах Ra [Phys. Rev. Lett. 114, 233002 (2015), однако известно, что молекулы гораздо лучше для этих целей)
- Ядра изотопов Ra имеют октупольную (pear-shape) деформацию (Physics World 2013 achievement)
- Кроме допплеровского охлаждения нет другого способа захватить RaF в ловушку (см. Таблицу), а значит выполнить прецизионные измерения

Холодные молекулы

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Method	Molecules	T	N
Photoassociation	Rb_2, Cs_2, He_2, H_2, Li_2, Na_2, K_2, Ca_2, KRb, RbCs, NaCs, LiCs, LiRb	30 μK	10^5
Feshbach/STIRAP	Li_2, Na_2, K_2, Rb_2, Cs_2, KRb	50 *n*K	$>10^5$
Buffer-gas cooling	CaH, CaF, VO, PbO, NH, CrH, MnH	400 *m*K	$>10^8$
Stark deceleration/ Trapping	NH_3, CO, OH, NH, SO_2, YbF, H_2CO, C_7H_5N	5 *m*K	10^6
Doppler cooling			

Участники

1. D.DeMille (Yale) SrF, J. Ye (JILA) YO
2. E.Hinds (Imperial College), CaF (http://arxiv.org/abs/1308.0421)
3. B. Odom (Northwestern Uni), AlH+
4. J.Doyle (Harvard Uni), SrOH
5. East China Normal University, MgF
6. Groningen University, SrF (RaF)

ПИЯФ+СПбГУ (RaF, RaOH, $UCaF_5$ …)

RaF

$$S_{00} = 0.999989$$

$$S_{01} = -0.001993$$

$$S_{02} = -0.001460$$

$$\Sigma S^2 = 0.999984$$

Нужен эксперимент по измерению франк-кондоновских факторов

Холодные молекулы

Таблица из статьи M. Schnell and G. Meijer, Angew. Chem. Int. Ed. ***48****, 6010 (2009)*

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Stark deceleration/ Trapping	NH_3, CO, OH, NH, SO_2, YbF, H_2CO, C_7H_5N	5 *m*K	10^6
Doppler cooling	SrF, YO, CaF, MgF, RaF	20 *m*K	300