Quantum Electrodynamics of the hydrogen molecule

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Searching for New Physics with light atoms and molecules

Any New Physics (BSM) would necessarily first manifest experimentally as a significant difference between experiments and theoretical predictions, but . . . .

The spectra of hydrogenic systems are being used for determination of physical constants and for precision tests of the fundamental interactions theory : H, μH, He$^+$, $e^+ e^-$, $\mu^+ e^-$, $\bar{p}$He$^+$, H_2^+, . . .

The 1S-2S transition in hydrogen is the most interesting candidate for high precision low-energy tests of SM Parthey *et al.* PRL 107,203001 (2011)

$$\nu(1S-2S)_{\mathrm{H}} = 2\,466\,061\,413\,187\,035(10)\ \mathrm{Hz}\ (4.2\times10^{-15})$$

The finite lifetime of excited states causes severe difficulties with interpretation of high precision spectroscopic results

Energy levels can be derived from QED theory using a few fundamental physical constants, $E = E(Ry, r_p, m/M, \alpha)$

The ultimate theoretical predictions are limited by the proton polarizabilities

Few-electron systems

The general purpose of our work is to bring the high accuracy achieved for hydrogenic energy levels to few-electron (light) atomic and molecular systems

There are (many) very narrow transitions that can be approached experimentally

Transition energies can in principle be calculated as accurately as $E(1S-2S)_H$, but the electron correlation makes calculations more difficult

Nonrelativistic quantum electrodynamics (NRQED), ($\alpha \approx 1/137$)

$$E(\alpha) = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \ldots, \qquad E^{(n)} \sim \alpha^n m$$

or

$$E(\alpha) = E_{\rm NR} + \alpha^2\, E_{\rm REL} + \alpha^3\, E_{\rm QED} + \alpha^{(n\geq 4)}\, E_{\rm HQED} + \ldots$$

The expansion coefficients can be expressed by expectation values of effective Hamiltonians with the nonrelativistic wave function. At present, $\alpha^7\, m$ is yet unknown in complete (only H-systems)

The basis of precise theoretical predictions are computational methods with explicitly correlated functions e.g. He, Li, hydrogen molecule

Hydrogen molecule

Many metastable levels with lifetime $10^5 - 10^6$ s. The first rotational state life time $\approx 10^{14}$ years

In addition, access to all six isotopic variants enables a robust verification of theory and measurements

Long-term goal: increasing accuracy from $\mathbf{10^{-3}\,cm^{-1}}$ (in 2009) up to $\mathbf{10^{-6}\,cm^{-1}}$ both experimentally and theoretically

Accuracy of 5 kHz ($1.6 \times 10^{-7}\mathrm{cm}^{-1}$) for the dissociation energy $D_0(H_2)$ will give r_p with 1% precision

$$\delta E_{\rm strong} = \langle \delta^3(r_{AB})\rangle\,(-2.389)\,{\rm fm}^2,\ \langle \delta^3(r_{AB})\rangle \approx 10^{-50}\,(m\,\alpha)^3$$

Hydrogen molecule can be calculated (almost) as accurately as H atom. The NRQED structure of operators can be obtained mostly from helium

Computational tools based on explicitly correlated (two-center, nonadiabatic) exponential (JC, KW, naJC, ECE) or gaussian functions (ECG, rECG, naECG)

Hydrogen molecule - some applications

Nuclear spin-spin coupling constant (in HD) is one of the best probe for BSM physics MP, Komasa, Pachucki PRL 95, 052506 (2018)

The most accurate $\mu_{d,t}$ from the NMR shielding

MP, Komasa, Pachucki PRA 92, 020501(R) (2015)

The rotational magnetic moment and the (nuclear) spin-rotation constant measured 60 years ago by *Ramsey et al.* still comprise the most precise experimental set of data and that since then no theoretical calculations achieved such an accuracy.

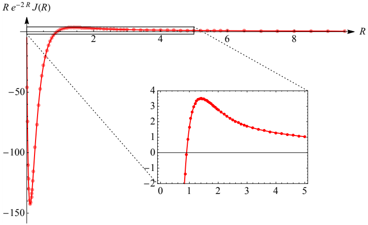
Spin-spin coupling $J(R)\,R\,e^{-2R}(\mathrm{Hz})$

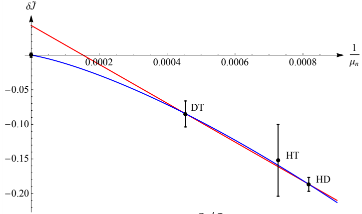
	HD	HT	DT
$J_{\mathrm{BO}}(R_e)$	$41.139\,2(3)$	$285.857(2)$	$43.880\,7(3)$
$\delta J(0K)$	$1.968\,0(9)$	$12.869(6)$	$1.554\,6(7)$
$\delta J(300K)$	$0.199\,5$	$1.391\,8$	$0.215\,3$
$J(300K)$	$43.306\,7(9)$	$300.117(6)$	$45.650\,6(9)$
$J_{\mathrm{exp}}(300K)$ [a]	$43.12(1)$	$299.06(36)$	$45.56(2)$
[b]	$43.115(9)$		

[a] P. Garbacz, *et al.*, J. Phys. Chem. A 120, 5549 (2016)
[b] Yu. I. Neronov and N. N. Seregin, JETP Letters **100**, 609 (2014)

Isotope dependence agrees with the behavior of $\sim 1/\mu_n$,.

The unique possibility to search for BSM physics

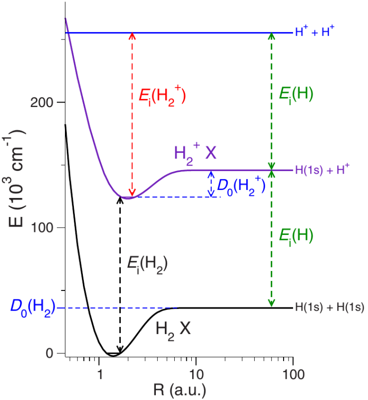




The fitted curve $A/\mu_n + B/\mu_n^{3/2}$ (blue), while the linear fit is $J_0 + C/\mu_n$ (red), with $J_0 = 0.043$ Hz

Dissociation energy - theory vs. experiments (2009/10)

	D_0/cm^{-1}	
	H_2	D_2
Experiment (1993)[1]	$36\,118.06(4)$	$36\,748.32(7)$
Experiment (2004)[2]	$36\,118.062(10)$	$36\,748.343(10)$
Experiment (2009/10)[3,4]	$36\,118.069\,62(37)$	$36\,748.362\,86(68)$
Theory (2009)[5]	$36\,118.069\,5(10)$	$36\,748.363\,3(9)$
Difference	$0.000\,1(11)$	$0.000\,4(11)$



Accuracy up to $10^{-5}\ \mathrm{cm}^{-1}$ for pure rotational transitions

The theoretical uncertainty of relativistic corrections in 2009 was underestimated at least by factor 4.

[1] E. E. Eyler, N. Melikechi, *Phys. Rev. A* **48**, R18 (1993);

[2] Y. Zang *et al.*, *Phys. Rev. Lett.* **92**, 203003 (2004);

[3] Liu, Salumbides, Hollenstein, Koelemeij, Eikema, Ubachs, Merkt, *JCP* **130**, 174306 (2009)

[4] Liu, Sprecher, Jungen, Ubachs, Merkt, *J. Chem. Phys.* **132**, 154301 (2010);

[5] Piszczatowski, Lach, Przybytek, Komasa, Pachucki, Jeziorski, *JCTC* **5**, 3039 (2009)

Expansion of energy levels (NAPT + NRQED, 2009)

$$
\begin{array}{lcccccccl}
E(\alpha,\beta) = & E_{\mathrm{BO}} & + & \alpha^2\, E_{\mathrm{REL}} & + & \alpha^3\, E_{\mathrm{QED}} & + & \alpha^4\, E_{\mathrm{HQED}} + \ldots \\
& + & & + & & + & & \vdots \\
& \beta\, E_{\mathrm{AD}} & & \alpha^2\,\beta\, E^{\mathrm{rec}}_{\mathrm{REL}} & & \alpha^3\,\beta\, E^{\mathrm{rec}}_{\mathrm{QED}} & & \\
& + & & \vdots & & \vdots & & \\
& \beta^2\, E_{\mathrm{NA}} & & & & & & \\
& \vdots & & & & & &
\end{array}
$$

Component		$D_0(H_2)/\mathrm{cm}^{-1}$
E_{BO}	the Born-Oppenheimer energy	$36112.592\,7(1)$
βE_{AD}	adiabatic correction	$+5.771\,1(1)$
$\beta^2 E_{\mathrm{NA}}$	nonadiabatic correction	$+0.434\,0(2)$
$\alpha^2 E_{\mathrm{REL}}$	relativistic correction	$-0.531\,8(5\times 4)$
$\alpha^3 E_{\mathrm{QED}}$	the leading QED correction	$-0.194\,8(3)$
$\alpha^4 E_{\mathrm{HQED}}$	higher order QED correction	$-0.001\,6(8)$
E	total	$36\,118.069\,5(10\times 4)$

Nonadiabatic nonrelativistic energies H_2

Four-particle basis of exponential functions (*naJC*) Komasa, Pachucki JCP 144, 164306 (2016); PCCP 20, 247 (2018); HD - PCCP 20, 26297 (2018); D_2 - PCCP (2019)

$$\psi(\vec{r}_1,\vec{r}_2)_{\{k\}} = e^{-\alpha\, R-\beta(\zeta_1+\zeta_2)}\, R^{k_0}\, r_{12}^{k_1}\, \eta_1^{k_2}\, \eta_2^{k_3}\, \zeta_1^{k_4}\, \zeta_2^{k_5}\,.$$

Ω	K	$E_{0,0}$	$D_{0,0}$
10	36 642	$-1.164\,025\,030\,822\,08$	$36\,118.797\,732\,723$
11	53 599	$-1.164\,025\,030\,870\,90$	$36\,118.797\,743\,437$
12	76 601	$-1.164\,025\,030\,880\,47$	$36\,118.797\,745\,538$
13	117 936	$-1.164\,025\,030\,883\,07$	$36\,118.797\,746\,108$
14	159 120	$-1.164\,025\,030\,883\,16$	$36\,118.797\,746\,129$
15	210 912	$-1.164\,025\,030\,883\,19$	$36\,118.797\,746\,135$
∞	∞	$-1.164\,025\,030\,883\,22(3)$	$36\,118.797\,746\,15(1)$

Arbitrary state can be obtained with a similar precision ($\sim 10^{-14}$)

Calculations of $\alpha^4 E_{\mathrm{HQED}}$ ($E^{(6)}$)

$$E^{(6)} = \langle H^{(6)} \rangle + \left\langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(4)} \right\rangle,$$

The second order contribution is sum

$$E_A = \left\langle H_A \frac{1}{(E_0 - H_0)'} H_A \right\rangle, \; E_C = \left\langle H_C \frac{1}{E_0 - H_0} H_C \right\rangle$$

E_A as well as $\langle H^{(6)} \rangle$ are separately divergent, but their sum is finite. We use the technique of dimensional regularization to eliminate these divergences from the matrix elements, eg. the hard three-photon exchange $d = 3 - 2\,\epsilon$ dimensions

$$H_H = \left(4 \ln m - \frac{1}{\epsilon} - \frac{39\,\zeta(3)}{\pi^2} + \frac{32}{\pi^2} - 6\,\ln(2) + \frac{7}{3}\right) \frac{\pi\,\alpha^3}{4\,m^2} \delta^d(r).$$

Elimination of $1/\epsilon$ divergences

The Breit-Pauli Hamiltonian

$$H_A = -\frac{p_1^4}{8\,m^3} - \frac{p_2^4}{8\,m^3} - \frac{\alpha}{2\,m^2}\,p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j + \frac{\pi\,\alpha}{m^2}\,\delta^3(r) + \frac{\pi\,Z_A\alpha}{2\,m^2}\,\delta^3(r_{1A}) + \frac{\pi\,Z_A\alpha}{2\,m^2}\,\delta^3(r_{2A}) + \frac{\pi\,Z_B\alpha}{2\,m^2}\,\delta^3(r_{1B}) + \frac{\pi\,Z_B\alpha}{2\,m^2}\,\delta^3(r_{2B}),$$

We use the transformation

$$H_A = H_A' + \{H_0 - E_0, Q\},$$

where

$$Q = -\frac{1}{4}\left(\frac{Z_A}{r_{1A}} + \frac{Z_B}{r_{1B}} + \frac{Z_A}{r_{2A}} + \frac{Z_B}{r_{2B}}\right) + \frac{1}{2\,r},$$

so that $E_A = E_A' + E_A''$, where

$$E_A' = \left\langle H_A'\,\frac{1}{(E_0 - H_0)'}\,H_A'\right\rangle,$$

$$E_A'' = \langle Q\,(E_0 - H_0)\,Q\rangle + 2\,\langle H_A\rangle\,\langle Q\rangle - \langle\{H_A\,,\,Q\}\rangle\,.$$

Regularized Breit-Pauli Hamiltonian

$$H'_A|\Phi\rangle = \Big\{-\frac{1}{2}(E_0 - V)^2 - p_1^i \frac{1}{2\,r}\left(\delta^{ij} + \frac{r^i\,r^j}{r^2}\right)p_2^j + \frac{1}{4}\vec{\nabla}_1^2\,\vec{\nabla}_2^2 + \frac{1}{2}(E - V)(V_1 + V_2) + \frac{1}{4}\vec{\nabla}_1(V_1 + V_2)\vec{\nabla}_1 + \frac{1}{4}\vec{\nabla}_2(V_1 + V_2)\vec{\nabla}_2\Big\}|\Phi\rangle,$$

where the action of $\vec{\nabla}_1^2\,\vec{\nabla}_2^2$ on Φ in the above is understood as a differentiation with omission of $\delta^3(r)$, and $V_i = 1/r_{iA} + 1/r_{iB}$

In order to satisfy the electron-electron cusp condition, we use rECG basis

$$\phi_{\Sigma^+} = \left(1 + \frac{r}{2}\right) e^{-a_{1A}\,r_{1A}^2 - a_{1B}\,r_{1B}^2 - a_{2A}\,r_{2A}^2 - a_{2B}\,r_{2B}^2 - a_{12}\,r_{12}^2}$$

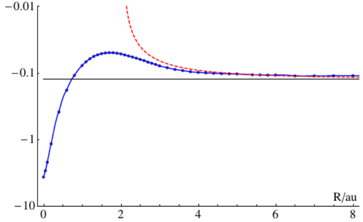
Recalculation of E_{REL} ($E^{(4,0)}$) correciton (BO) MP, Komasa and Pachucki PRA 95, 052506 (2017)

1024 ECG + direct, a.u.	1024 *r*ECG + regularization, a.u.
$\mathbf{-0.205\,682(8)}$	$\mathbf{-0.205\,688\,526(7)}$

Contributions to $E^{(6)}$ at $R = 1.4$ au.

$\alpha^6\, m$	$H_2(\Sigma^+)$
E'_Q	$0.688\,40(16)$
E'_H	$-0.043\,832$
E'_A	$-0.641\,4(5)$
E_C	$-0.059\,54(4)$
Subtotal	$-0.056\,4(6)$
E_{R1}	$9.254\,583$
E_{R2}	$0.142\,233$
E_{LG}	$0.258\,811$
Total	$9.599\,3(6)$
$-2\,E_D(\mathrm{H})$	$0.125\,000$
$-2\,E_{R1}(\mathrm{H})$	$-6.123\,245$
$-2\,E_{R2}(\mathrm{H})$	$-0.109\,212$
$E^{(6)}(\mathrm{H}_2) - 2\,E^{(6)}(\mathrm{H})$	$3.491\,8(6)\,\alpha^6\, m$

FIG. 1. Non-logarithmic photon exchange contribution $E'_Q + E'_A + E_C + E'_H$ as a function of the inter-nuclear distance R. The horizontal line is located at $-1/8$, which is twice the atomic hydrogen value, and the dashed curve shows the $0.529\,947\,904/R^2 - 1/8$ asymptotics, which is obtained from the small R expansion of the Casimir-Polder potential [20].



MP, Czachorowski, Komasa and Pachucki PRL 117, 263002 (2016)

Relativistic correction in nonadiabatic approach

Nonadiabatic ECG basis

$$\phi = r_{01}^{n_{01}}\, e^{-a_{01} r_{01}^2 - a_{02} r_{02}^2 - a_{03} r_{03}^2 - a_{12} r_{12}^2 - a_{13} r_{13}^2 - a_{23} r_{23}^2}$$

$$\begin{aligned} H_{\rm rel} \;=\; & -\frac{1}{8}(p_2^4 + p_3^4) + \frac{\pi}{2}\sum_{X,a}\left(1 + \frac{\delta_s}{m_X^2}\right)\delta^3(r_{Xa}) \\ & +\pi\,\delta^3(r) - \frac{1}{2}\,p_2^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\, r^j}{r^3}\right)p_3^j \\ & +\frac{1}{2}\sum_{X,a}\frac{1}{m_X}p_X^i\left(\frac{\delta^{ij}}{r_{Xa}} + \frac{r_{Xa}^i\, r_{Xa}^j}{r_{Xa}^3}\right)p_a^j \\ & +\frac{1}{2}\,\frac{1}{m_0\, m_1}p_0^i\left(\frac{\delta^{ij}}{r_{01}} + \frac{r_{01}^i\, r_{01}^j}{r_{01}^3}\right)p_1^j \end{aligned}$$

Basis	δ $D_0(H_2)/\mathrm{cm}^{-1}$
128	$-0.531\,427\,54$
256	$-0.531\,194\,19$
512	$-0.531\,206\,99$
1024	$-0.531\,212\,77$
2048	$-0.531\,214\,84$
∞	$-0.531\,215\,6(5)$

MP, Spyszkiewicz, Komasa and Pachucki PRL 121, 073001 (2018)

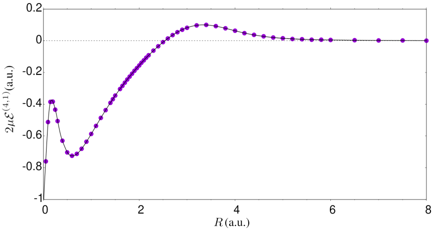
In calculations we applied combination of naECG and na-rECG (e-e cusp) functions

Nonadiabatic relativistic correction (NAPT)

$$E^{(4,1)} = \frac{1}{\mu_n}\Big(\langle\vec{\nabla}_R\psi_{\rm rel}|\vec{\nabla}_R\psi\rangle - \langle\psi_{\rm rel}|\vec{\nabla}^2_{\rm el}\psi\rangle + \frac{1}{4}\langle\psi|Q_{\rm M}\psi\rangle\Big)$$

$$|\psi_{\rm rel}\rangle = \frac{1}{(E_0 - H_0)'}\,H_{\rm A}|\psi\rangle$$

Q_M represents the first order orbit-orbit terms



Czachorowski, MP, Komasa and Pachucki PRA 98, 052506 (2018)

The above formulas expand to complex expressions, demanding computationally eg. up to the third order in PT

Calculations are based on ECG as well as rECG (e-e cusp) bases.

The uncertainty $2\cdot 10^{-6}$ cm^{-1} for $D_0(H_2)$ from neglected nonadiabatic effects $O(\sqrt{\beta})$.

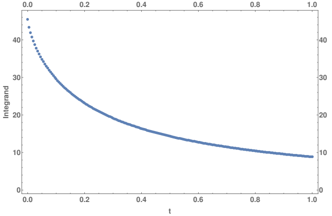
QED correction in nonadiabatic approach

$$E^{(5)} = -\frac{2\mathcal{D}}{3\,\pi}\ln k_0 - \frac{7}{6\,\pi}\left\langle \frac{1}{r_{23}^3} + \frac{m}{m_p}\sum_{a,x}\frac{1}{r_{ax}^3} + \frac{m^2}{m_p^2}\frac{1}{r_{01}^3}\right\rangle_\epsilon + \left(\frac{164}{15} + \frac{14}{3}\ln\alpha\right)\langle\delta^3(r_{23})\rangle$$
$$+ \frac{4}{3}\left\{\frac{19}{30} + \ln(\alpha^{-2}) + \frac{m}{4\,m_p}\left[\frac{62}{3} + \ln(\alpha^{-2})\right] + \frac{m^2}{m_p^2}\left[\ln\left(\frac{m_p}{m}\right) + \ln(\alpha^{-2}) + 4\right]\right\}\sum_{a,x}\langle\delta^3(r_{ax})\rangle$$

Bethe logarithm - Schwartz method

$$\ln k_0 = \frac{1}{\mathcal{D}}\int_0^1 dt\,\frac{f(t) - f_0 - f_2\,t^2}{t^3}$$

$$f(t) = \left\langle \vec{J}\,\frac{k}{k + H - E}\,\vec{J}\right\rangle, \qquad t = \frac{1}{\sqrt{1 + 2\,k}}$$



N	E	$\ln k_0$
128	−1.164 023 669 155	3.016 586 1
256	−1.164 024 987 878	3.018 137 0
512	−1.164 025 027 334	3.018 258 91
1024	−1.164 025 030 593	3.018 301 73
2048	−1.164 025 030 843	3.018 303 90
∞	−1.164 025 030 86(3)	3.018 304 9(15)

MP, Komasa, Czachorowski and Pachucki PRL 122, 103003 (2019)

Dissociation energy for H_2 in cm^{-1} (present)

Contribution	$D_{0,0}$	$D_{0,1}$	$(0,1) \to (0,0)$	
$E^{(2)}$	$36\,118.797\,746\,10(3)$	$36\,000.312\,485\,66(2)$	$118.485\,260\,44(4)$	naJC
$E^{(4)}$	$-0.531\,215\,6(5)$	$-0.533\,799\,2(5)$	$0.002\,583\,55(2)$	naECG, + ECG
$E^{(5)}$	$-0.194\,910\,43(15)$	$-0.193\,887\,7(11)$	$-0.001\,022\,7(11)$	naECG, + ECG
$E^{(6)}$	$-0.002\,067(6)$	$-0.002\,058(6)$	$-0.000\,008\,9$	naECG, + ECG
$E^{(6)}_{\rm sec}$	$0.000\,009\,2$	$0.000\,009\,1$	$0.000\,000\,1$	ECG
$E^{(7)}$	$0.000\,101(25)$	$0.000\,101(25)$	$0.000\,000\,5(1)$	
$E^{(4)}_{\rm FS}$	$-0.000\,031$	$-0.000\,031$	$-0.000\,000\,2$	
Total[a]	$36\,118.069\,632(26)$	$35\,999.582\,820(26)$	$118.486\,812\,7(11)$	
Exp.	$36\,118.069\,62(37)$[b]	$35\,999.582\,894(25)$[c]	$118.486\,8(1)$	
Diff.	$-0.000\,01(37)$	$0.000\,074(36)$	$0.000\,0(1)$	
Exp.	$36\,118.069\,45(31)$[d]	$35\,999.582\,834(11)$[e] $\leftarrow$ *new!*		
Diff.	$-0.000\,18(31)$	$0.000\,014(28)$		

[a] MP, Komasa, Czachorowski and Pachucki PRL 122, 103003 (2019)

[b] Liu, Salumbides, Hollenstein, Koelemeij, Eikema, Ubachs, and Merkt, JCP 130, 174306 (2009)
[c] Cheng, Hussels, Niu,Bethlem, Eikema, Salumbides, Ubachs, Beyer, Holsch, J. Agner PRL. 121, 013001 (2018)
[d] Altmann, Dreissen, Salumbides, Ubachs, Eikema, PRL 120, 043204 (2018).
[e] Holsch, Beyer, Salumbides, Eikema, Ubachs, Jungen and Merkt, PRL. 122, 103002 (2019)

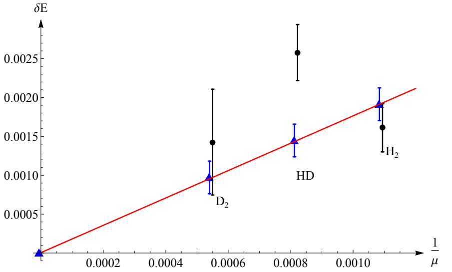
Dissociation energy for isotopologues in cm^{-1}

TABLE IV. Theoretical predictions for the dissociation energy budget for the ground level of H_2. $E^{(6)}_{\rm sec}$ is a second order correction due to relativistic BO potential; $E_{\rm FS}$ is the finite nuclear size correction with $r_p = 0.84087(39)$ fm [28]. All the energy entries are given in cm^{-1}.

Contribution	D_2	T_2	HD	HT	DT
$E^{(2)}$	36 749.090 989 81(1)	37 029.224 867 15(1)	36 406.510 890 20(1)	36 512.928 009 26(1)	36 882.009 843 46(1)
$E^{(4)}$	−0.528 206 05(9)	−0.526 750 0(2)	−0.529 887 5(2)	−0.529 377 9(2)	−0.527 523 6(3)
$E^{(5)}$	−0.198 256(3)	−0.199 736(4)	−0.196 440(4)	−0.197 006(5)	−0.198 958(5)
$E^{(6)}$	−0.002 096(6)	−0.002 110(6)	−0.002 080(6)	−0.002 085(6)	−0.002 103(6)
$E^{(6)}_{\rm sec}$	0.000 009 4	0.000 009 4	0.000 009 3	0.000 009 3	0.000 009 4
$E^{(7)}$	0.000 103(25)	0.000 103(25)	0.000 102(25)	0.000 102(25)	0.000 103(25)
$E^{(4)}_{\rm FS}$	−0.000 202	−0.000 139(6)	−0.000 116	−0.000 084(3)	−0.000 171(3)
Total[a]	36 748.362 342(26)	37 028.496 245(27)	36 405.782 478(26)	36 512.199 568(26)	36 881.281 200(26)
Exp.	36 748.362 86(68)[b]		36 405.783 66(36)[c]		
Diff.	0.000 52(68)		0.001 18(36)		

MP, Spyszkiewicz, Komasa and Pachucki in preparition

Experiments
Sprecher, Liu, Jungen, Ubachs, Merkt, JCP 133, 111102 (2010)
Liu, Sprecher, Jungen, Ubachs, Merkt, JCP 132, 154301 (2010)



Conclusions

- Currently, the main D_0 uncertainty of ca. $25 \cdot 10^{-6}$ cm^{-1} (0.75 MHz) from $E^{(7)}$
- Possible determination r$_p$ with 1% accuracy at $1.6 \cdot 10^{-7}$ cm^{-1} (5 kHz)

$$E(\mathrm{H}_2, \mathrm{IP}) = D_0(\mathrm{H}_2) + E(\mathrm{H}, \mathrm{IP}) - D_0(\mathrm{H}_2^+)$$

- Significant differences for HD between experiments and theory
- Looking for BSM physics, the difference between theoretical predictions and experimental results should be convincingly established
- Accurate calculatoins of the hyperfine couplings, the spin-spin coupling etc. are planed soon that will be a challenge to new experiments.