# Fine structure and hyperfine structure of some excited states of helium

B.C. Gou<sup>a</sup>, F. Wang<sup>b</sup>, and X.L. Wu<sup>c</sup>

Department of Physics, Beijing Institute of technology, Beijing 100081, P.R. China

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**Abstract.** The fine structure and the hyperfine structure for some singly-excited and doubly-excited states of helium atom are calculated using Rayleigh-Ritz variational method with multi-configuration-interaction wave functions. The calculated results of the fine structure for the Rydberg series are in good agreement with other theoretical and experimental data. The hyperfine parameters and the hyperfine coupling constants of <sup>3</sup>He are also obtained for this system.

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## **1** Introduction

Helium is the simplest coulomb three-body system that exhibits strong electron-electron correlation. Both experimental measurements of energies and spectra in helium and the corresponding theoretical calculations are fundamental problems in atomic physics. The large fine structure intervals of the 1s2p <sup>3</sup>P<sup>o</sup> state of helium is ideal for investigating the fine structure constant  $\alpha$  and for testing QED to this two-electron system. Many experimental and theoretical investigations have been achieved very high precision for the 1s2p <sup>3</sup>P<sup>o</sup> state [1–17]. Experimentally, the development of laser spectroscopy and microwave measurement made advantageous to measure fine structure to very high accuracy. Shiner et al. [1] measured the Lamb shift and fine structure of the 2s  ${}^{3}S-2p$   ${}^{3}P^{o}$  transition in helium using laser excitation of an atomic beam. George et al. [2] achieved the most precise result of 2  ${}^{3}P^{o}$  fine structure of helium in microwave measurement. Theoretically, Lewis et al. [9] predicted the fine structure splittings of the J = 1 to J = 0 interval of the 1s2p <sup>3</sup>P<sup>o</sup> state by including the major part of the second-order contribution to the fine structure. Drake et al. [10–13] substantially improved the precision of the fine structure calculations for this state, with computational uncertainties less than 1 kHz, by including all known terms of order  $\alpha^5$  a.u.  $(\alpha^7 mc^2)$  arising from the electron-electron interaction and recoil corrections of order  $\alpha^4 \mu/M$  a.u. Using the variational wavefuntions constructed by doubled Hylleraas basis sets, Drake [15] provided essentially exact results for

the entire singly-excited spectrum of helium. However, to our knowledge, few data have been reported for the fine structure of the singly-excited and doubly-excited states of helium atom.

In this paper, the fine structure and the hyperfine structure for some singly-excited and doubly-excited states of helium are calculated using Rayleigh-Ritz variational method with multi-configuration-interaction wave functions. The hyperfine parameters and the hyperfine coupling constants are also explored for this system. The available data should be very useful in better understanding the experimental spectra in the future.

#### 2 Theory

The non-relativistic Hamiltonian for helium atom is given in atomic units by

$$H_0 = \sum_{i=1}^{2} \left[ -\frac{1}{2} \nabla_i^2 - \frac{2}{r_i} \right] + \frac{1}{r_{12}}$$
(1)

The basic wave function for the two-electron system can be written as

$$\Psi_b(1,2) = A \sum_i C_i \phi_{n(i),l(i)}(R) Y_{l(i)}^{LM}(\Omega) \chi_{SS_z}$$
(2)

where A is the antisymmetrization operator and the radial basis function is Slater orbital

$$\phi_{n(i),l(i)}(R) = \prod_{j=1}^{2} r_j^{n_j} \exp(-\alpha_j r_j).$$
(3)

<sup>&</sup>lt;sup>a</sup> e-mail: goubing@sina.com

<sup>&</sup>lt;sup>b</sup> e-mail: fwang@bit.edu.cn

<sup>&</sup>lt;sup>c</sup> e-mail: xlwu@sina.com

The angular part is

$$Y_{l(i)}^{LM}(\Omega) = \sum_{m_j} \langle l_1 l_2 m_1 m_2 | LM \rangle \prod_{j=1}^2 Y_{l_j m_j}(\Omega_j) \quad (4)$$

where

$$Y_{lm}(\theta,\varphi) = (-1)^m \left[ \frac{(2l+1)(1-m)!}{4\pi(1+m)!} \right]^{1/2} \times P_l^m(\cos\theta) \exp(\mathrm{i}m\varphi) \quad (5)$$

and  $P_l^m(\cos \theta)$  is an associated Legendre polynomial.

A different set of  $\alpha_j$  is used for each angular parts  $[l_1, l_2]$ . The linear parameters  $C_i$  and the nonlinear parameters  $\alpha_j$  are determined in the energy optimization processes.

The total energy is further improved by including the relativistic corrections and mass polarization effect. The explicit expressions of these perturbation operators are given in reference [18], they will not be repeated here. Then the total energy becomes  $E_{\text{total}} = E_b + \Delta E_{\text{rel}}$ .

The fine-structure perturbation operators are given by

$$H_{\rm FS} = H_{\rm SO} + H_{\rm SOO} + H_{\rm SS} \tag{6}$$

where the spin-orbit, spin-other-orbit, and spin-spin operators are

$$H_{\rm SO} = \frac{Z\alpha^2}{2} \sum_{i=1}^2 \frac{\mathbf{l}_i \cdot \mathbf{s}_i}{r_i^3} \tag{7}$$

$$H_{\text{SOO}} = -\frac{\alpha^2}{2} \sum_{\substack{i,j=1\\i\neq j}}^2 \left[ \frac{1}{r_{ij}^3} (\mathbf{r}_i - \mathbf{r}_j) \times \mathbf{P}_i \right] . (\mathbf{s}_i + 2\mathbf{s}_j) \quad (8)$$

$$H_{\rm SS} = \alpha^2 \sum_{\substack{i,j=1\\i \prec j}}^2 \frac{1}{r_{ij}^3} \left[ \mathbf{s}_i \cdot \mathbf{s}_j - \frac{3(\mathbf{s}_i \cdot \mathbf{r}_{ij})(\mathbf{s}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right].$$
(9)

The  $\mathbf{l}_i$  and  $\mathbf{s}_i$  are the orbital and the spin angular momentum of the *i*th electron. To calculate the fine structure splitting, the LSJ coupling scheme is used:

$$\Psi_{LSJJ_Z} = \sum_{S_Z, L_Z} \langle LSL_Z S_Z | JJ_Z \rangle \Psi_b(1, 2).$$
(10)

The fine-structure energy levels are calculated by firstorder perturbation theory:

$$(\Delta E_{\rm FS})_J = \langle \Psi_{LSJJ_Z} | H_{\rm SO} + H_{\rm SOO} + H_{\rm SS} | \Psi_{LSJJ_Z} \rangle.$$
(11)

For a two-electron system, the hyperfine interaction Hamiltonian can be represented as follows [20,21]:

$$H_{\rm hfs} = \sum_{k=1}^{\infty} T^{(k)} M^{(k)} \tag{12}$$

where  $T^{(k)}$  and  $M^{(k)}$  are spherical tensor operators of rank k in the electronic and nuclear space, respectively. The

k = 1 term represents the magnetic-dipole interaction between the magnetic field generated be the electrons and nuclear magnetic dipole moments, the k = 2 term the electric quadrupole interaction between the electric field gradient from the electrons and the non-spherical charge distribution of the nucleus. The higher-order contribution terms are much smaller and can often be neglected.

In the non-relativistic framework, the electronic tensor operators can be written as:

$$T^{(1)} = \frac{\alpha^2}{2} \sum_{i=1}^{2} \left[ 2g_l r_i^{-3} l_i^{(1)} - \sqrt{10} g_s \left\{ s_i^{(1)} C_i^{(2)} \right\}^{(1)} r_i^{-3} + \frac{8\pi}{3} g_s s_i^{(1)} \delta(\mathbf{r}_i) \right]$$
(13)

and

$$T^{(2)} = -\sum_{i=1}^{2} r_i^{-3} C_i^{(2)} \tag{14}$$

where  $\alpha$  is the fine structure constants,  $g_l = (1 - m_e/M)$ and  $g_s = 2.0023193$  are the orbital the electron spin g factor, respectively.  $\delta$  is the three-dimensional delta function. M is the nuclear mass. The tensor  $C_i^{(2)}$  is connected to the spherical harmonics  $Y_{lm}$  by

$$C_m^{(l)} = \sqrt{\frac{4\pi}{2l+1}} Y_{lm}(\theta,\varphi). \tag{15}$$

The hyperfine interaction couples the electronic angular momenta  $\mathbf{J}$  and the nuclear angular momenta  $\mathbf{I}$  to a total angular momentum  $\mathbf{F} = \mathbf{I} + \mathbf{J}$ . The uncoupling hyperfine constants  $a_C$ ,  $a_{SD}$ ,  $a_l$ , and  $b_q$  are defined as follows [20,21]:

$$a_{C} = \left\langle \gamma LSLS \left| \sum_{i=1}^{2} 8\pi \delta^{3}(\mathbf{r}_{i}) s_{0}(i) \right| \gamma LSLS \right\rangle$$
(Fermi contact) (16)

$$a_{SD} = \left\langle \gamma LSLS \left| \sum_{i=1}^{2} 2C_0^{(2)}(i) s_0(i) r_i^{-3} \right| \gamma LSLS \right\rangle$$
(spin-dipolar) (17)

$$a_{l} = \left\langle \gamma LSLS \left| \sum_{i=1}^{2} l_{0}(i) r_{i}^{-3} \right| \gamma LSLS \right\rangle \quad \text{(orbital)} \quad (18)$$
$$b_{q} = \left\langle \gamma LSLS \left| \sum_{i=1}^{2} 2C_{0}^{(2)}(i) r_{i}^{-3} \right| \gamma LSLS \right\rangle \quad \text{(electric quadrupole)} \quad (19)$$

and the coupling hyperfine constants  $A_J$  and  $B_J$  are de-

$$A_{J} = \frac{\mu_{I}}{I} \frac{1}{\left[J(J+1)(2J+1)\right]^{1/2}} \left\langle \gamma J \left| \left| T^{(1)} \right| \right| \gamma J \right\rangle \quad (20)$$

fined as follows:

$$B_{j} = 2Q \left[ \frac{2J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right]^{1/2} \left\langle \gamma J \left\| T^{(2)} \right\| \gamma J \right\rangle$$
(21)

where  $\mu_I$  is the nuclear magnetic moment. Q is the nuclear electric quadrupole moment.

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		$\Delta E_J \; (\mu { m a.u.})$						
States	$E_{\rm CG}$	J = L + 1	J = L	J=L-1	$\nu_{3-2}$	$\nu_{2-1}$	$\nu_{1-0}$	Source
1s2p <sup>3</sup> P <sup>o</sup>	770521.69	-0.659	-0.304	4.206		-0.0779	-0.9895	This work
	770521.69	-0.655	-0.307	4.196		-0.0765	-0.9881	Drake [15]
						-0.0764	-0.9879	Drake [13]
						-0.0764	-0.9879	Zhang and Drake [12]
						-0.0766	-0.9875	Hijikata [26]
						-0.0764	-0.9879	Pchucki [14]
						-0.0764	-0.9879	Exp. $[1]$
							-0.9879	Exp. $[2]$
						-0.0764	-0.9879	Exp. $[3]$
						-0.0764	-0.9879	Exp. $[4, 6]$
						-0.0764	-0.9879	Exp. $[7]$
						-0.0764	-0.9879	Exp. [8]
$1s3p$ $^{3}P^{o}$	845618.17	-0.188	-0.076	1.168		-0.0245	-0.2731	This work
	845610.18	-0.182	-0.181	1.152		-0.0220	-0.2707	Drake [15]
1s4p <sup>3</sup> P <sup>o</sup>	871375.61	-0.079	-0.028	0.481		-0.0112	-0.1119	This work
	871368.26	-0.074	-0.033	0.470		-0.0090	-0.1103	Drake [15]
$1s5p$ $^{3}P^{o}$	883159.05	-0.042	-0.012	0.247		-0.0066	-0.0570	This work
	883140.67	-0.037	-0.017	0.236		-0.0045	-0.0554	Drake [15]
1s6p <sup>3</sup> P <sup>o</sup>	889543.28	-0.023	-0.005	0.132		-0.0039	-0.0301	This work
	889484.47	-0.021	-0.010	0.135		-0.0026	-0.0317	Drake [15]
$2p^2 {}^3\mathrm{Pe}$	2193289.61	4.480	-4.150	-9.960		1.8932	1.2760	This work
$2p3p$ $^{3}P^{e}$	2335973.64	4.400	-4.330	-9.010		1.9165	1.0270	This work
$2p4p$ $^{3}P^{e}$	2367920.52	4.428	-4.400	-8.937		1.9372	0.9955	This work
$2p5p$ $^{3}P^{e}$	2381534.32	4.437	-4.424	-8.915		1.9444	0.9855	This work
$2p6p$ $^{3}P^{e}$	2388627.91	4.442	-4.434	-8.906		1.9477	0.9813	This work
$1s3d$ $^{3}\mathrm{D^{e}}$	848058.65	-0.048	-0.532	0.165	-0.0034	-0.0434		This work
	848058.65	-0.046	-0.035	0.166	-0.0025	-0.0442		Drake [15]
$1s4d$ $^{3}\mathrm{D^{e}}$	872404.73	-0.020	-0.013	0.070	-0.0015	-0.0183		This work
	872404.73	-0.020	-0.014	0.070	-0.0012	-0.0185		Drake [15]
$1s5d$ $^{3}\mathrm{D^{e}}$	883673.61	-0.010	-0.007	0.036	-0.0008	-0.0094		This work
	883673.61	-0.010	-0.007	0.036	-0.0006	-0.0095		Drake [15]
$1s6d$ $^{3}\mathrm{D^{e}}$	889793.21	-0.006	-0.004	0.021	-0.0005	-0.0054		This work
	889793.21	-0.006	-0.004	0.021	-0.0004	-0.0055		Drake [15]
$2p3d$ $^{3}D^{o}$	2344460.22	2.907	-1.452	-4.364	0.9565	0.6392		This work
$2p4d$ $^{3}D^{o}$	2371110.79	2.948	-1.471	-4.427	0.9696	0.6488		This work
$2p5d$ $^{3}\mathrm{D^{o}}$	2383081.68	2.959	-1.477	-4.442	0.9734	0.6505		This work
$2p6d$ $^{3}D^{o}$	2389498.99	2.962	-1.480	-4.445	0.9746	0.6508		This work

**Table 1.** Center-of-gravity term energies  $E_{CG}$  ( $\mu a.u.$ ), fine structure corrections  $\Delta E_J$  (in  $\mu a.u.$ ) and fine structure splittings  $\nu_{J-J'}$  (in cm<sup>-1</sup>) for some triplet states in helium.

#### 3 Results and discussion

In this work, ten Rydberg series of helium, 1sns <sup>1,3</sup>S<sup>e</sup>, 1snp <sup>1,3</sup>P°, 1snd <sup>1,3</sup>D°, 2pnp <sup>1,3</sup>P°, and 2pnd <sup>1,3</sup>D° states with n = 2-6, are studied. The fine structure and hyperfine structure for these Rydberg systems are calculated using Rayleigh-Ritz variational method with accurate multiconfiguration-interaction wave functions constructed from Slater basis sets. The electron correlation effects between the two electrons are large. Many relevant angular and spin couplings are important for the energy. In order to get the high quality wave function, the number of angular-spin components in the wave functions ranges from 5 to 10, and the number of linear parameters ranges from 85 to 253. The angular series  $[l_1, l_2]$  with more than  $1.0 \times 10^{-5}$  a.u. energy contribution are included in  $\Psi_b$ , and l is up to 9, as the energy contribution from set with l > 9 is small and negligible.

Table 1 shows the center-of-gravity energies in this work are in good agreement with the theoretical data of Drake [15]. This indicates that the precision of our calculation is sufficiently high in this two-electron system. Comparisons have been made between this work and Drake [15] for the fine structure correction to the center-of-gravity term energy of the 1*snl* <sup>3</sup>P<sup>o</sup>, and <sup>3</sup>D<sup>e</sup> states. Our calculation results of the fine structure corrections are almost the same as that of Drake [15]. This shows that our method is effective in the calculations of the fine structure corrections. The fine structure splittings for this system are also given in Table 1. The 1s2p <sup>3</sup>P<sup>o</sup> state is an excellent system to test QED and to measure fine structure constant, many high precision measurements and calculations have been achieved [1–14]. The calculation of the fine structure splittings in 1s2p <sup>3</sup>P<sup>o</sup> state has been completed to order  $\alpha^7 mc^2$  by Drake [13]. Compared with these high precision

Resonances	$a_c$	$a_{ m SD}$	$a_l$	$b_q$
1s2s <sup>3</sup> S <sup>e</sup>	33.17192			
$1s3s$ ${}^{3}S^{e}$	32.28694			
$1s4s$ ${}^{3}S^{e}$	32.10615			
$1s5s$ ${}^{3}\mathrm{S}^{\mathrm{e}}$	32.01638			
$1s6s$ ${}^{3}S^{e}$	32.02034			
1s2p <sup>1</sup> P <sup>o</sup>			0.03825	-0.01214
1s3p <sup>1</sup> P <sup>o</sup>			0.01126	-0.00363
1s4p <sup>1</sup> P <sup>o</sup>			0.00476	-0.00153
1s5p <sup>1</sup> P <sup>o</sup>			0.00248	-0.00079
1s6p <sup>1</sup> P <sup>o</sup>			0.00145	-0.00046
$2p3p$ $^{3}P^{e}$			0.17962	0.07185
2p4p <sup>1</sup> P <sup>e</sup>			0.17136	0.06854
2p5p <sup>1</sup> P <sup>e</sup>			0.16816	0.06726
2p6p <sup>1</sup> P <sup>e</sup>			0.16785	0.06714
1s2p <sup>3</sup> P°	31.62570	-0.01402	0.06933	-0.02804
1s3p <sup>3</sup> P <sup>o</sup>	31.87949	-0.04118	0.02001	-0.00824
1s4p <sup>3</sup> P°	31.94746	-0.00169	0.00818	-0.00338
1s5p <sup>3</sup> P <sup>o</sup>	31.96391	-0.00083	0.00404	-0.00167
1s6p <sup>3</sup> P <sup>o</sup>	31.97688	-0.00039	0.00189	-0.00077
$2p^2 {}^3\mathrm{P}^{\mathrm{e}}$		0.04355	0.21777	0.08711
$2p3p$ $^{3}P^{e}$		0.03506	0.17531	0.07012
2p4p <sup>3</sup> P <sup>e</sup>		0.03399	0.16993	0.06797
2p5p <sup>3</sup> P <sup>e</sup>		0.03364	0.16822	0.06729
2p6p <sup>3</sup> P <sup>e</sup>		0.03350	0.16751	0.06700
2p3d <sup>1</sup> D <sup>o</sup>			0.11430	0.12437
2p4d <sup>1</sup> D <sup>o</sup>			0.11251	0.13009
$2p5d$ $^{1}D^{o}$			0.11177	0.13178
2p6d <sup>1</sup> D <sup>o</sup>			0.11148	0.13250
$1s3d$ $^{1}\mathrm{D^{e}}$			0.00499	-0.00121
$1s4d$ $^{1}\mathrm{D^{e}}$			0.00211	-0.00061
$1s5d$ $^{1}\mathrm{D^{e}}$			0.00108	-0.00031
$1s6d$ $^{1}\mathrm{D^{e}}$			0.00062	-0.00018
$2p3d$ $^{3}D^{o}$		0.06523	0.11462	0.13047
$2p4d$ $^{3}D^{o}$		0.06606	0.11250	0.13212
$2p5d$ $^{3}D^{o}$		0.06637	0.11183	0.13275
$2p6d$ $^{3}D^{o}$		0.06649	0.11151	0.13299
1s3d <sup>3</sup> D <sup>e</sup>	31.98370	-0.00072	0.00501	-0.00144
$1s4d^{3}\mathrm{D^{e}}$	31.98610	-0.00030	0.00212	-0.00061
$1s5d$ $^{3}\mathrm{D^{e}}$	31.98722	-0.00016	0.00108	-0.00031
1s6d <sup>3</sup> D <sup>e</sup>	31.98759	-0.00009	0.00062	-0.00018

Table 2. Hyperfine parameters of some single-excited and double-excited states for  ${}^{3}$ He (in a.u.).

theoretical and experimental data, as Table 1 shows, our results of the fine structure splittings are in reasonable agreement with those of Drake [15]. For example, the fine structure splittings  $\nu_{2-1}$  and  $\nu_{1-0}$  are -0.0015 cm<sup>-1</sup> and -0.0183 cm<sup>-1</sup> for 1.54d <sup>3</sup>D state in this work, respectively. And the corresponding results of Drake [15], using double basis set with Hylleraas basis function, are -0.0012 cm<sup>-1</sup> and  $-0.0185 \,\mathrm{cm}^{-1}$ , respectively. For easy comparison with the results of Drake [15] and experimental data [1-8], we transferred our results to term energies relative to ground state in eV according to the following principle: 1 a.u. = 27.20767 eV, and the energy of the ground state is 79.0056 eV [24]. We transferred the results of Drake [15] from MHz to  $\mu$ a.u. or cm<sup>-1</sup> according to the following principle: 1 a.u. = 219444.54 cm<sup>-1</sup>. Furthermore, we calculated the fine structure of the doubly-excited

 $2lnl~^3\mathrm{P^e},$  and  $^3\mathrm{D^o}$  states. To our knowledge, no calculations have been reported for the fine structure of this doubly-excited state system. Our reliable theoretical results should be useful for studying the spectra in the future.

The hyperfine structure is caused by the interaction between the electrons and the electromagnetic multipole moments of the nucleus, sensitive to the correlation effects between electrons and the relativistic corrections. The hyperfine structure of 2  ${}^{3}P^{\circ}$  levels of  ${}^{3}He$  has been a subject of experimental and theoretical interest in atomic physics for a long time [25–29]. Recently, the hyperfine splitting of 2  ${}^{3}S_{1}$  state in  ${}^{3}He$  is explored by Pachucki [30]. A very large second-order correction due to the Fermi interaction have been found in their work. Tables 2 and 3 give the hyperfine parameters and the hyperfine coupling constants

Resonances –	I = 3	$\frac{AJ}{I-2}$	I-1
	0 = 0	0 - 2	0 = 1
1s2s <sup>3</sup> S <sup>e</sup>			-4.49443
1s3s <sup>3</sup> S <sup>e</sup>			-4.37453
1s4s <sup>3</sup> S <sup>e</sup>			-4.35003
1s5s <sup>3</sup> S <sup>e</sup>			-4.34193
1s6s <sup>3</sup> S <sup>e</sup>			-4.33840
1s2p <sup>1</sup> P <sup>o</sup>			-1.55276(-2)
1s3p <sup>1</sup> P <sup>o</sup>			-4.57232(-3)
1s4p <sup>1</sup> P <sup>o</sup>			-1.93333(-3)
1s5p <sup>1</sup> P <sup>o</sup>			-1.00639(-3)
$1s6p$ $^{1}P^{o}$			-5.86835(-4)
$2p3p$ $^{1}P^{e}$			-7.29127(-2)
$2p4p$ $^{1}P^{e}$			-6.95572(-2)
$2p5p$ $^{1}P^{e}$			-6.82588(-2)
$2p6p$ $^{1}P^{e}$			-6.81350(-2)
1s2p <sup>3</sup> P <sup>o</sup>		-2.15369	-2.17079
1s3p <sup>3</sup> P <sup>o</sup>		-2.16288	-2.16791
1s4p <sup>3</sup> P <sup>o</sup>		-2.16558	-2.16764
1s5p <sup>3</sup> P <sup>o</sup>		-2.16603	-2.16705
1s6p <sup>3</sup> P <sup>o</sup>		-2.16656	-2.16704
$2p^2 {}^3\mathrm{P^o}$		-5.30509(-2)	5.93094(-5)
2p3p <sup>3</sup> P <sup>e</sup>		-4.27064(-2)	4.77446(-5)
2p4p <sup>3</sup> P <sup>e</sup>		-4.13974(-2)	4.62811(-5)
2p5p <sup>3</sup> P <sup>e</sup>		-4.09792(-2)	4.58136(-5)
2p6p <sup>3</sup> P <sup>e</sup>		-4.08069(-2)	4.56210(-5)
2p3d <sup>1</sup> D°		-2.31993(-2)	
2p4d <sup>1</sup> D <sup>o</sup>		-2.28348(-2)	
2p5d <sup>1</sup> D <sup>o</sup>		-2.26855(-2)	
2p6d <sup>1</sup> D <sup>o</sup>		-2.26271(-2)	
1s3d <sup>1</sup> D <sup>e</sup>		-1.01304(-3)	
1s4d <sup>1</sup> D <sup>e</sup>		-4.27647(-4)	
1s5d <sup>1</sup> D <sup>e</sup>		-2.18655(-4)	
1s6d <sup>1</sup> D <sup>e</sup>		-1.26719(-4)	
$2p3d$ $^{3}D^{o}$	-2.43477(-2)	-3.91885(-3)	1.15071(-2)
$2p4d$ $^{3}D^{o}$	-2.41731(-2)	-3.36418(-3)	1.27410(-2)
$2p5d$ $^{3}\mathrm{D^{o}}$	-2.41240(-2)	-3.17616(-3)	1.31681(-2)
$2p6d$ $^{3}D^{\circ}$	-2.40974(-2)	-3.09421(-3)	1.33497(-2)
$1s3d$ $^{3}\mathrm{D^{e}}$	-1.44506	-7.23259(-1)	2.16468
$1s4d$ $^{3}\mathrm{D^{e}}$	-1.44483	-7.22724(-1)	2.16602
$1s5d$ $^{3}\mathrm{D^{e}}$	-1.44476	-7.22540(-1)	2.16652
1s6d <sup>3</sup> D <sup>e</sup>	-1.44473	-7.22455(-1)	2.16673

Table 3. Hyperfine coupling constants of some single-excited and double-excited states for <sup>3</sup>He (in GHz).

 $A_J$  for  $1sns^{1,3}$ S<sup>e</sup>,  $1snp^{1,3}$ P<sup>o</sup>,  $1snd^{1,3}$ D<sup>e</sup>,  $2pnp^{1,3}$ P<sup>e</sup>, and  $2pnd^{1,3}$ D<sup>o</sup> states in <sup>3</sup>He. In this calculation, high precise wave functions are used. We studied the hyperfine structure parameters: Fermi contact  $a_c$ , the spin-dipolar  $a_{\rm SD}$ , the orbital  $a_l$ , and the electric quadrupole  $b_q$ . In this work, Q = 0.0b,  $\mu_I = -2.127625$  nm, and I = 1/2 are taken from reference [19]. To our knowledge, few data of the hyperfine parameters  $a_c$ ,  $a_{\rm SD}$ ,  $a_l$ ,  $b_q$ , and hyperfine coupling constants  $A_J$  have been reported for this system of <sup>3</sup>He in the literature.

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### References

- D. Shiner, R. Dixson, P. Zhao, Phys. Rev. Lett. 72, 1802 (1994)
- M.C. George, L.D. Lombardi, E.A. Hessels, Phys. Rev. Lett. 87, 173002 (2001)
- F. Minardi, G. Bianchini, P. Cancio Pastor, G. Giusfredi, F.S. Pavone, M. Inguscio, Phys. Rev. Lett. 82, 1112 (1999)
- 4. C.H. Storry, E.A. Hessels, Phys. Rev. A 58, R8 (2000)
- J. Castillega, D. Livingston, A. Sanders, D. Shiner, Phys. Rev. Lett. 84, 4321 (2000)
- C.H. Storry, M.C. George, E.A. Hessels, Phys. Rev. Lett. 84, 3274 (2000)
- 7. J. Wen, Ph.D. thesis, Harvard University, 1996 (unpublished)

- F.M.J. Pichanick, R.D. Swift, C.E. Johnson, V.W. Hughes, Phys. Rev. 169, 55 (1968)
- 9. M.L. Lewis, P.H. Serafino, Phys. Rev. A 18, 867 (1978)
- 10. G.W.F. Drake, Z.C. Yan, Phys. Rev. A 46, 2378 (1992)
- Z.C. Yan, G.W.F. Drake, Bull. Am. Phys. Soc. 38, 1127 (1993)
- 12. T. Zhang, G.W.F. Drake, Phys. Rev. A 54, 4882 (1996)
- 13. G.W.F. Drake, Can. J. Phys. 80, 1195 (2002)
- 14. K. Pachucki, J. Sapirstein, J. Phys. B **33**, 5297 (2000)
- G.W.F. Drake, Atomic Molecular and Optical Physics Handbook (American Institute of Physics, New York, 1996), Chap. 11
- X.-X. Guan, B.-W. Li, Z.-W. Wang, Chin. Phys. Lett. 19, 654 (2002)
- F. Miardi, M. Inguscio, Gregory Breit Centennial Symposium, New Haven, CT USA, 22–26 Oct. 1999 (Singapore, World Scientific 2001), pp. 35-51
- 18. H.Y. Yang, K.T. Chung, Phys. Rev. A 51, 3621 (1995)
- 19. P. Rayhavan, At. Data Nucl. Data Tables 42, 181 (1989)

- 20. A. Hibbert, Rep. Prog. Phys. 38, 1217 (1975)
- J. Carlsson, P. Jonsson, C.F. Fischer, Phys. Rev. A 46, 2420 (1992)
- 22. X.-X. Guan, Z.-W. Wang, Eur. Phys. J. D 2, 21 (1998)
- L.H. Han, B.C. Gou, H.Y. Hu, F. Wang, Int. J. Mod. Phys. C 13, 397 (2002)
- A.A. Radzig, B.M. Smirnov, *Reference Data on Atoms, Molecules, and Ions* (Springer Series in Chemical Physics 31, Springer-Verlag Berlin, 1985), Chaps. 5 and 7
- E.A. Hinds, J.D. Prestage, F.M.J. Pichanick, Phys. Rev. A 32, 2615 (1985)
- 26. K. Hijikata, K. Ohtsuki, J. Phys. Soc. Jap. 57, 4141 (1988)
- 27. K. Ohtsuki, K. Hijikata, J. Phys. Soc. Jap. 57, 4150 (1988)
- W.R. Johnson, K.T. Cheng, D.R. Plante, Phys. Rev. A 55, 2728 (1997)
- E. Riis, A.G. Sinclair, O. Poulsen, G.W.F. Drake, W.R.C. Rowley, A.P. Levick, Phys. Rev. A 49, 207 (1994)
- 30. K. Pachucki, J. Phys. B 34, 3357 (2001)