Relativistic and quantum electrodynamics corrections to the binding energies of the $(J=1,\nu=1)$ states of $dd\mu$ and $dt\mu$

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(Received 8 February 1990)

The relativistic shift, including the corrections to the binding energy due to vacuum polarization, the hyperfine splitting, and nuclear finite-size effects have been calculated for the $(J=1,\nu=1)$ states of $dd\mu$ and $dt\mu$. The corrections have been determined by first-order perturbation theory using the nonrelativistic wave functions determined by Alexander and Monkhorst [S. A. Alexander and H. J. Monkhorst, Phys. Rev. A **38**, 26 (1988)]. The results show rapid convergence with basis-set size. The overall convergence of the calculations is better than 0.01 meV. The accuracy of the total correction to the binding energies is estimated to be ± 0.5 meV.

I. INTRODUCTION

Ever since Vesman suggested the possibility of the resonant formation of $dd\mu$ via the loosely bound state with quantum numbers $J=1$ and $\nu=1$,[1] the theoretical study of loosely bound states in both $dd\mu$ and $dt\mu$ has greatly intensified, resulting in molecular wave functions and binding energies with increasingly higher precision. The nonrelativistic binding energies for these states is now known to an accuracy of 0.1 meV.[2-4] The relativistic corrections to the binding energies, however, exceed the required accuracy by several orders of magnitude. It therefore becomes imperative to include relativistic effects at least to lowest order in perturbation theory. In addition, due to the much smaller Bohr radius of the muonic system, the small distance corrections to the Coulombic potential originating from radiative corrections (QED) as well as finite size and internal degrees of freedom—such as nuclear polarizability—of the nuclei may rise well above the desired level of accuracy (0.1 meV). In this work the relativistic shift, the hyperfine splitting, the correction to the Coulombic potential due to finite nuclear sizes and vacuum polarization are evaluated perturbatively using the very accurate wave functions obtained by Alexander and Monkhorst.[2] The results converge rapidly with basis-set size to well within the required accuracy of 0.1 meV.

II. THEORY

A. Basis set

The nonrelativistic wave functions used in this work were computed by Alexander and Monkhorst.[2] The wave functions are expanded in a basis set of explicitly correlated Slater-type geminals. The exponential parameters in these geminals are calculated using random tempering formulas. Both the linear and the nonlinear parameters are variationally optimized so as to minimize the total energy. For the $J=1$ states of $dt\mu$ the wave function has the form

$$\Psi_{dt\mu,J=1}=\sum_{i=1}^{K}(c_i z_1+\tilde{c}_i z_2)e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_{12})}, \tag{1}$$

where r_1 and r_2 are the distances between the muon and nuclei 1 and 2, respectively, $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, and $z_1=r_1\cos\theta_1$ and $z_2=r_2\cos\theta_2$. For $dd\mu$ one has

$$\Psi_{dd\mu,J=1}=\sum_{i=1}^{K}c_i(z_1 e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_{12})} - z_2 e^{-(\beta_i r_1+\alpha_i r_2+\gamma_i r_{12})}). \tag{2}$$

If we rewrite both wave functions in the form

$$\Psi=z_1\chi_1+z_2\chi_2 \tag{3}$$

we find for $dt\mu$

$$\chi_1=\sum_{i=1}^{K}c_i e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_{12})},$$
$$\chi_2=\sum_{i=1}^{K}\tilde{c}_i e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_{12})}, \tag{4}$$

and for $dd\mu$

$$\chi_1=\sum_{i=1}^{K}c_i e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_{12})},$$
$$\chi_2=-\sum_{i=1}^{K}c_i e^{-(\beta_i r_1+\alpha_i r_2+\gamma_i r_{12})}. \tag{5}$$

B. Relativistic three-particle Hamiltonian

The relativistic Hamiltonian for three-particle systems including only electromagnetic interactions can be approximated as

$$H_{\rm rel}=\sum_{n=0}^{1}H^{(n)}, \tag{6}$$

with $H^{(n)}=O(\alpha^{2n})$. We will demand that $H^{(0)}$ represents the nonrelativistic Hamiltonian (corrected for nuclear finite-size effects) and that this relativistic Hamiltonian contains no three-particle interactions. In such a case the relativistic correction terms can be derived from the rela-

tivistic scattering amplitude by solving the Lippman-Schwinger equation for the scattering amplitude.[5–7] The nuclear finite-size effects can be incorporated into the Hamiltonian by means of form factors.[8,9] For particles of spin $s \leq \frac{3}{2}$ the general form of the electromagnetic current matrix element (involving the form factors of the particles) has been found by Glaser and Jakšić.[10] This method will yield a Breit-Pauli Hamiltonian for the three-particle system.[11,12] We can write

$$H^{(n)}=T^{(n)}+U^{(n)} , \tag{7}$$

with

$$T^{(n)}=\sum_i T_i^{(n)} \tag{8}$$

and

$$U^{(n)}=\sum_{i<j} U_{ij}^{(n)} , \tag{9}$$

where i and j number the particles. The operators $T_i^{(n)}$ are the kinetic energy and the relativistic recoil or mass-velocity operator, and have the forms

$$T_i^{(0)}=\frac{p_i^2}{2m_i} \tag{10}$$

and

$$T_i^{(1)}=-\frac{\alpha^2 p_i^4}{8m_i^3} . \tag{11}$$

The potentials $U_{ij}^{(n)}$ depend only on the positions, momenta, and spins of particles i and j:

$$U_{ij}^{(n)}=U_{ij}^{(n)}(\mathbf{r}_{ij},\mathbf{p}_{ij},\mathbf{P}_{ij},\mathbf{s}_i,\mathbf{s}_j) . \tag{12}$$

Here we have used the notations

$$\begin{aligned} \mathbf{r}_{ij}&=\mathbf{r}_j-\mathbf{r}_i , \\ \mathbf{p}_{ij}&=\frac{m_i\mathbf{p}_j-m_j\mathbf{p}_i}{m_i+m_j} , \\ \mathbf{P}_{ij}&=\mathbf{p}_i+\mathbf{p}_j , \end{aligned} \tag{13}$$

where m_i, $\mathbf{r}_i$, $\mathbf{p}_i$, and $\mathbf{s}_i$ are the mass, position, momentum, and spin of particle i, respectively. The potential $U_{ij}^{(0)}$ is—as required—the Coulomb potential, which is corrected for the inclusion of the nuclear finite-size effects

$$U_{ij}^{(0)}=\frac{Z_iZ_j}{r_{ij}}+U_{ij}^{(\mathrm{NFS})} , \tag{14}$$

where

$$U_{ij}^{(\mathrm{NFS})}=-\frac{Z_iZ_j g_{(1)}(r_{ij})}{r_{ij}} . \tag{15}$$

The function $g_{(1)}(r_{ij})$ expresses the effect of the finite size of the particles on the interparticle Coulomb potential (see Appendix A). The first-order correction to the potential can be written as a sum of a number of terms

$$U_{ij}^{(1)}=U_{ij}^{(D)}+U_{ij}^{(\mathrm{RMC})}+U_{ij}^{(\mathrm{VP})}+U_{ij}^{(F)}+U_{ij}^{(\mathrm{SO})}+U_{ij}^{(T)}+U_{ij}^{(Q)} , \tag{16}$$

with (the units $\hbar=e=1$ are used throughout)

$$U_{ij}^{(D)}=\alpha^2\left[\hat{g}_{(2)}(r_{ij})\frac{s_i}{2s_i+1}\frac{(Z_i-\mu_i/s_i)Z_j}{2m_i^2}+\hat{g}_{(2')}(r_{ij})\frac{s_j}{2s_j+1}\frac{Z_i(Z_j-\mu_j/s_j)}{2m_j^2}\right] \tag{17}$$

the Darwin term (here μ_i is the magnetic moment of particle i in units $e\hbar/2M_ic$),

$$U_{ij}^{(\mathrm{RMC})}=-\frac{Z_iZ_j\alpha^2}{2m_im_jr_{ij}}\left[(\mathbf{p}_i\cdot\mathbf{p}_j)+\frac{[\mathbf{r}_{ij}(\mathbf{r}_{ij}\cdot\mathbf{p}_i)\mathbf{p}_j]}{r_{ij}^2}\right] \tag{18}$$

the relativistic mass correction, which expresses the relativistic retardation of the interparticle Coulomb interaction,[12]

$$U_{ij}^{(\mathrm{VP})}=\frac{2Z_iZ_j\alpha}{3\pi r_{ij}}\int_1^\infty dx\frac{(x^2-1)^{1/2}(1+1/2x^2)}{x^2}e^{-2\gamma x r_{ij}} \tag{19}$$

the Uehling potential,[13] with $\gamma=m_ec/\hbar$,

$$U_{ij}^{(F)}=-\tfrac{1}{6}\alpha^2\hat{g}_{(3)}(r_{ij})\left[\frac{\mu_i}{m_is_i}\right]\left[\frac{\mu_j}{m_js_j}\right](\mathbf{s}_i\cdot\mathbf{s}_j) \tag{20}$$

the Fermi contact term,

$$U_{ij}^{(\mathrm{SO})}=\alpha^2\left[-\frac{Z_iZ_j}{2m_i^2}\frac{(\mathbf{r}_{ij}\times\mathbf{p}_i)\cdot\mathbf{s}_i}{r_{ij}^3}+\frac{Z_iZ_j}{2m_j^2}\frac{(\mathbf{r}_{ij}\times\mathbf{p}_j)\cdot\mathbf{s}_j}{r_{ij}^3}-\frac{Z_i\mu_j}{2m_{ij}m_js_j}\frac{(\mathbf{r}_{ij}\times\mathbf{p}_{ij})\cdot\mathbf{s}_j}{r_{ij}^3}-\frac{Z_j\mu_i}{2m_{ij}m_is_i}\frac{(\mathbf{r}_{ij}\times\mathbf{p}_{ij})\cdot\mathbf{s}_i}{r_{ij}^3}\right] \tag{21}$$

the spin-orbit interaction,

$$U_{ij}^{(T)}=-\frac{\alpha^2}{4r_{ij}^3}\left[\frac{\mu_i}{m_is_i}\right]\left[\frac{\mu_j}{m_js_j}\right]\times\left[\frac{3(\mathbf{r}_{ij}\cdot\mathbf{s}_i)(\mathbf{r}_{ij}\cdot\mathbf{s}_j)}{r_{ij}^2}-(\mathbf{s}_i\cdot\mathbf{s}_j)\right] \tag{22}$$

the spin-spin dipole interaction, and

$$U_{ij}^{(Q)}=\frac{Z_iQ_j\alpha^2}{2r_{ij}^3}\left[\frac{3(\mathbf{r}_{ij}\cdot\mathbf{s}_j)^2}{r_{ij}^2}-s_j^2\right]+\frac{Z_jQ_i\alpha^2}{2r_{ij}^3}\left[\frac{3(\mathbf{r}_{ij}\cdot\mathbf{s}_i)^2}{r_{ij}^2}-s_i^2\right] \tag{23}$$

the quadrupole interaction (Q_i being the particle i electric quadrupole moment). In addition, we will use the operators $U_{ij}^{(\bar{D})}$ and $U_{ij}^{(\bar{F})}$, which represent the Darwin and Fermi corrections without nuclear finite-size effects. The operators $T_i^{(1)}$, $U_{ij}^{(\mathrm{NFS})}$, $U_{ij}^{(D)}$, $U_{ij}^{(\mathrm{RMC})}$, and $U_{ij}^{(\mathrm{VP})}$ are

TABLE I. Physical constants used in this calculation. Masses are given in units of m_e, magnetic moments in units of $e\hbar/2M_ic$, and the quadrupole moment in units of fm^2.

Constant	Value			
	General constants			
$1/\alpha$	137.035 989 5			
Rydberg	13.605 698 1			
	Particle Properties			
Property	muon	proton	deuteron	triton
Mass	206.7686	1836.1515	3670.481	5496.918
Magnetic moment	1.00117	2.792 846	1.7139	9.819
Quadrupole moment			0.286	

TABLE II. Proton, deuteron, and triton form-factor parameters. Λ's are given in MeV/c. Values are taken from Ref. 26. For symbols, see Appendix A.

Particle	Nuclear form factor	w_{ijs}	Λ_{ijs}	l_{ijs}
p	Dirac	0.789	852	2
		0.211	2095	2
	Pauli	0.437	770	3
		0.563	1194	3
d	Charge	0.350	374	5
		0.663	707	5
		−0.013	1980	5
	Magnetic	0.389	381	5
		0.611	756	5
	Quadrupole	0.561	444	5
		0.439	798	5
t	Dirac	1.654	701	5
		−0.654	848	5
	Pauli	1.533	522	3
		−0.533	697	3

the spin-independent terms and the remaining terms in (16) are the spin-dependent terms. The first set of operators causes a shift in the binding energy, the last one causes the hyperfine splitting. The quadrupole interaction will only be included for particles with $s_i \geq 1$. Note that the finite-size effects are only included in the δ-function-type contributions, i.e., the Darwin and the Fermi contact terms, and in the Coulomb potential. All other contributions are one order of magnitude smaller than the δ terms. The small corrections to these due to the nuclear finite size can be neglected.[14]

III. PRACTICAL CONSIDERATIONS

The matrix elements of the operators in the preceding section can all be expressed in closed analytical form. However, the expectation values do not converge well. This difficulty is due to numerical instability of the analytical expressions and is caused by large cancellation effects in the elementary matrix elements themselves. In contrast to the numerical instability caused by the near-linear dependency of the geminal basis set encountered in the determination of the nonrelativistic wave function,[2] these instabilities cannot be removed by performing the calculations in 128-bit precision. The only terms that can be calculated analytically in our basis set are the δ-function terms and those which show δ-function-like behavior, like the nuclear finite-size correction integrals. The determination of the vacuum polarization contribution is done with a mixed technique in which three of the four integrations are performed analytically and one is done numerically (see Appendix B). All other contributions to the relativistic corrections for the muonic molecules are determined by numerical integration. The technical details of this integration are discussed by Bakalov[15] and Alexandrov and Bakalov.[16] All of the numerical integrations have been performed in 64-bit precision.

Tables I and II give the numerical values of the physical constants used in the calculations.[17]

IV. RESULTS

Tables III–VI give results of our calculations for dtμ, Tables VII–XII for ddμ. The hyperfine splitting levels are given with respect to the weighted center of the spectrum. The corrections to the binding energy are calculated using the definition $\Delta\varepsilon_{11}=\Delta E_{11}^{\text{molecule}}-\Delta E_{10}^{\text{atom}}$. All re-

TABLE III. Convergence with basis-set size K of the contributions to the relativistic shift for dtμ ($J=1,\nu=1$) in meV.

K	$\bar{D}$	D	RMC	$T^{(1)}$	VP	NFS	Total
100	−2.49	−2.44	−0.07	4.14	15.92	3.11	20.67
200	−2.26	−2.26	−0.38	3.49	15.87	11.40	28.03
300	−2.34	−2.35	−0.45	3.60	16.41	13.37	30.58
400	−2.48	−2.47	−0.45	3.84	16.77	13.29	30.98
500	−2.46	−2.47	−0.45	3.83	16.72	13.31	30.94
600	−2.38	−2.39	−0.45	3.69	16.60	13.38	30.83
800	−2.42	−2.41	−0.45	3.72	16.61	13.33	30.80
1000	−2.41	−2.41	−0.45	3.73	16.62	13.31	30.80
1200	−2.41	−2.42	−0.44	3.74	16.61	13.30	30.79
1400	−2.41	−2.42	−0.44	3.74	16.61	13.29	30.78

TABLE IV. Convergence with basis-set size K of the hyperfine splitting for dtμ ($J=1,\nu=1$) in meV.

	State quantum numbers ($\mathcal{J}IS$)									
K	$0\,\frac{3}{2}\,1$	$2\,\frac{3}{2}\,1$	$1\,\frac{3}{2}\,1$	$1\,\frac{1}{2}\,0$	$1\,\frac{1}{2}\,1$	$2\,\frac{1}{2}\,1$	$0\,\frac{1}{2}\,1$	$1\,\frac{3}{2}\,2$	$3\,\frac{3}{2}\,2$	$2\,\frac{3}{2}\,2$
100	−164.82	−164.78	−164.74	52.53	53.63	53.80	53.80	55.87	56.15	56.21
200	−148.38	−148.31	−148.22	43.96	46.36	46.77	46.85	51.72	52.39	52.52
300	−144.01	−143.95	−143.84	41.38	44.44	44.93	45.05	50.60	51.25	51.52
400	−143.73	−143.67	−143.57	41.26	44.33	44.83	44.95	50.51	51.16	51.45
500	−143.71	−143.64	−143.54	41.25	44.33	44.81	44.93	50.50	51.16	51.44
600	−143.84	−143.77	−143.67	41.30	44.37	44.86	44.98	50.54	51.20	51.48
800	−143.87	−143.80	−143.70	41.32	44.39	44.88	44.99	50.55	51.20	51.48
1000	−143.89	−143.83	−143.73	41.33	44.40	44.89	45.00	50.56	51.21	51.49
1200	−143.90	−143.84	−143.74	41.34	44.41	44.89	45.01	50.56	51.21	51.49
1400	−143.91	−143.85	−143.74	41.34	44.41	44.89	45.01	50.56	51.21	51.49

TABLE V. Convergence with basis-set size K of the hyperfine splitting for dtμ ($J=1,\nu=1$) in meV (including nuclear finite-size effects).

	State quantum numbers ($\mathcal{J}IS$)									
K	$0\,\frac{3}{2}\,1$	$2\,\frac{3}{2}\,1$	$1\,\frac{3}{2}\,1$	$1\,\frac{1}{2}\,0$	$1\,\frac{1}{2}\,1$	$2\,\frac{1}{2}\,1$	$0\,\frac{1}{2}\,1$	$1\,\frac{3}{2}\,2$	$3\,\frac{3}{2}\,2$	$2\,\frac{3}{2}\,2$
100	−162.88	−162.84	−162.80	51.91	53.00	53.17	53.17	55.21	55.48	55.54
200	−147.43	−146.54	−146.45	43.17	45.80	46.21	46.30	51.09	51.66	51.89
300	−142.29	−142.22	−142.12	40.89	43.91	44.39	42.52	49.98	50.63	50.91
400	−142.02	−141.95	−141.85	40.78	43.80	44.30	44.42	49.90	50.55	50.83
500	−141.99	−141.93	−141.82	40.76	43.80	44.28	44.40	49.89	50.55	50.83
600	−141.99	−141.93	−141.82	40.76	43.80	44.28	44.40	49.89	50.55	50.83
800	−142.16	−142.10	−142.00	40.84	43.86	44.35	44.47	49.94	50.59	50.87
1000	−142.18	−142.11	−142.01	40.85	43.87	44.35	44.47	49.94	50.59	50.88
1200	−142.18	−142.12	−142.02	40.85	43.87	44.36	44.48	49.94	50.60	50.88
1400	−142.19	−142.12	−142.02	40.85	43.88	44.36	44.48	49.95	50.60	50.88

TABLE VI. Converged hyperfine splitting and mixing amplitudes for dtμ ($J=1,\nu=1$) in meV ($K=1400$). These numbers include the nuclear finite-size effects.

			amplitudes $\beta_{I,S}$			
$\mathcal{J}$	IS	$\varepsilon_{\mathcal{J},I,S}$	$\beta_{1/2,0}$	$\beta_{1/2,1}$	$\beta_{3/2,1}$	$\beta_{3/2,2}$
0	$\frac{3}{2}\,1$	−142.19	0.000 00	0.559 62	0.828 75	0.000 00
	$\frac{1}{2}\,1$	44.48	0.000 00	0.828 75	−0.559 62	0.000 00
1	$\frac{3}{2}\,1$	−142.02	−0.001 14	0.557 67	0.830 06	−0.002 26
	$\frac{1}{2}\,0$	40.85	0.995 36	−0.064 96	0.045 54	−0.053 19
	$\frac{1}{2}\,1$	43.88	0.084 59	0.824 06	−0.553 28	0.087 47
	$\frac{3}{2}\,2$	49.95	0.045 78	−0.074 72	0.052 97	0.994 74
2	$\frac{3}{2}\,1$	−142.12	0.000 00	0.556 49	0.830 85	−0.001 24
	$\frac{1}{2}\,1$	44.36	0.000 00	0.830 82	−0.556 49	−0.008 16
	$\frac{3}{2}\,2$	50.88	0.000 00	0.007 47	−0.003 51	0.999 97
3	$\frac{3}{2}\,2$	50.60	0.000 00	0.000 00	0.000 00	1.000 00

TABLE VII. Total relativistic correction to dtμ binding energy in meV.

Contributions to relativistic shift	
Darwin correction	−2.42
Relativistic mass correction	−0.44
Recoil	3.74
Total relativistic shift	0.86
Vacuum polarization (Uehling potential)	16.61
Nuclear finite-size correction to Coulomb potential	13.29
Lowest hyperfine state	35.22
Total correction	65.98
Additional corrections	
Deuteron polarizability[a]	−2.2
Molecular finite-size effect[b]	0.29
Total correction to binding energy	64.1

[a]Value from Bakalov (Ref. 7).
[b]Value from Scrinzi and Szalewicz (Ref. 29).

sults are in meV. As can be seen from these tables, all numerical values converge to well within the desired accuracy of 0.1 meV. For ddμ the convergence is much faster than for dtμ. This trend is analogous to the convergence of the binding energy[2] and interparticle distances.[18]

The influence of the inclusion of nuclear finite size on the Darwin correction is seen to be almost negligible. The effect on the hyperfine splitting is larger, i.e., it reduces the total splitting by almost 2 meV for dtμ and 0.4 meV for ddμ. However, the atomic hyperfine splitting is also reduced, and therefore the correction to the binding energy is only slightly reduced by nuclear finite-size effects. For dtμ the correction to the binding energy due to the hyperfine splitting is changed ≈ 1 meV by nuclear finite-size effects and hence has to be taken into account in order to arrive at the desired accuracy.

Previous calculations of the interparticle distances for dtμ ($J=1, \nu=1$) indicate that it can be considered as a tμ atom with a loosely bound deuteron.[18] Therefore the main contribution to the hyperfine splitting should come from the tμ Fermi interaction. The grouping of the hyperfine states—three levels with a total weight of 9 centered around −142.1 meV and seven levels with a total weight of 27 centered around 47.4 meV—indicates the dominant role of this interaction. Interestingly, the ratio of these averages is 1:3 as expected from the atomic Landé rule, but their value is reduced by 20%. The additional splitting is mainly due to the dμ Fermi interaction and to the spin-orbit coupling.

TABLE IX. Convergence with basis-set size K of the hyperfine splitting for ddμ ($J=1, \nu=1$) in meV.

	State quantum numbers (δIS)				
K	$\frac{3}{2}\,1\,\frac{1}{2}$	$\frac{1}{2}\,1\,\frac{1}{2}$	$\frac{1}{2}\,1\,\frac{3}{2}$	$\frac{3}{2}\,1\,\frac{3}{2}$	$\frac{5}{2}\,1\,\frac{3}{2}$
100	−16.32	−16.09	7.74	8.01	8.32
200	−16.36	−16.13	7.75	8.04	8.34
300	−16.35	−16.12	7.74	8.04	8.33
400	−16.35	−16.12	7.74	8.04	8.33
500	−16.35	−16.11	7.74	8.04	8.33
600	−16.35	−16.11	7.74	8.04	8.33
800	−16.34	−16.11	7.74	8.04	8.33
1000	−16.35	−16.11	7.74	8.04	8.33

For ddμ the situation is more complicated, but similar relations can be observed. Here the splitting is also grouped in two structures, which are separated by approximately half the atomic hyperfine splitting.

The dtμ hyperfine structure is naturally described according to the following particle spin coupling scheme: $\mathbf{F}=\mathbf{s}_t+\mathbf{s}_\mu$, $\mathbf{s}=\mathbf{F}+\mathbf{s}_d$; while the ddμ hyperfine structure better fits the coupling scheme $\mathbf{I}=\mathbf{s}_{d_1}+\mathbf{s}_{d_2}$, $\mathbf{s}=\mathbf{I}+\mathbf{s}_\mu$.

Comparison with other recent calculations[19–21] is made in Table XIII. The agreement with the results from Bakalov and co-workers is striking. It is a consequence of the application of the same operators in the calculation of the corrections. The wave function they employed is different, but apparently has the same global quality as the one we have used here. The difference with the scalar correction calculated by Myint *et al.*[20] is mainly due to the use of a different charge form factor for tritium.

Recently Myint *et al.*[20] argued that the triton charge form factors used by Bakalov are based on outdated results and are not very accurate. Use of more recent experimental data[22] resulted in a nuclear finite-size correction for dtμ that differed as much as 2.9 meV from the results obtained by Bakalov using form-factor data derived from experiments reported in 1967 by Griffy and Schiff.[23]

TABLE VIII. Convergence with basis-set size K of the contributions to the relativistic shift for ddμ ($J=1, \nu=1$) in meV.

K	$\tilde{D}$	D	RMC	$T^{(1)}$	VP	NFS	Total
100	−1.09	−1.06	0.48	2.16	11.00	−1.83	10.75
200	−0.83	−0.80	0.46	1.71	8.56	−1.40	8.53
300	−0.91	−0.88	0.46	1.86	8.68	−1.53	8.59
400	−0.91	−0.88	0.46	1.86	8.64	−1.52	8.56
500	−0.91	−0.88	0.46	1.87	8.65	−1.53	8.57
600	−0.91	−0.88	0.46	1.87	8.66	−1.53	8.58
800	−0.91	−0.89	0.46	1.87	8.66	−1.54	8.56
1000	−0.91	−0.89	0.46	1.87	8.66	−1.54	8.56

TABLE X. Convergence with basis-set size K of the hyperfine splitting for ddμ ($J=1, \nu=1$) in meV (including nuclear finite-size effects).

	State quantum numbers ($\mathcal{J}IS$)				
K	$\frac{3}{2}\,1\,\frac{1}{2}$	$\frac{1}{2}\,1\,\frac{1}{2}$	$\frac{1}{2}\,1\,\frac{3}{2}$	$\frac{3}{2}\,1\,\frac{3}{2}$	$\frac{5}{2}\,1\,\frac{3}{2}$
100	−16.11	−15.88	7.63	7.91	8.22
200	−16.14	−15.91	7.64	7.93	8.23
300	−16.13	−15.90	7.64	7.93	8.22
400	−16.13	−15.90	7.64	7.93	8.22
500	−16.13	−15.90	7.64	7.93	8.22
600	−16.13	−15.90	7.64	7.93	8.22
800	−16.13	−15.90	7.64	7.93	8.22
1000	−16.13	−15.90	7.64	7.93	8.22

Using the more recent form factors and fitting them to generalized dipole functions—see Appendix A—indeed changes the value of the nuclear finite-size correction from the old value of 13.3 meV to a value much closer to the number obtained by Myint *et al.*, e.g., 10.9 meV. The difference between their value and ours is caused by a considerable deviation of the contribution of the finite size of the deuteron. In Ref. 20 the dμ contribution to the total energy of dtμ (11) is quoted to be 4.2 meV, whereas we find for the same contribution a value of 4.7 meV. This is consistent with the difference in the atomic corrections for dμ: they find 213 meV, we find 215 meV. The reason for the latter discrepancy is unclear, but might be due to the use of a theoretical form factor by Myint *et al.*[20] rather than the experimental one we use.[24]

The reliability of the calculated corrections is more difficult to assess, since it requires knowledge of the size of higher-order corrections as well as information about the errors of the experimental parameters, such as nuclear form factors and deuteron polarizability. Because the higher-order corrections will be approximately two orders of magnitude smaller than the first-order effects, we expect these not to alter the present results significantly. The uncertainty in the size of the deuteron polarizability effect limits the reliability of the current value of the total correction to the binding energy to 0.5 meV. The deuteron polarizability correction to the binding energy of dtμ obtained by using a phenomenological model fitted to experimental data by Bakalov was −2.2 meV. Kamimura obtained a more accurate value by using first-principles methods. The value he obtained is −2.0 meV.[25] However, he argues that the correction due to the triton polarizability is approximately 0.4 meV and should hence be included. In addition, the error bars on the physical constants in Table I as well as the remaining uncertainty in the nuclear finite-size effects are such that further improvement of the results beyond the level of 0.1 meV can only be obtained provided more accurate values of these experimental constants have been determined.

TABLE XI. Converged hyperfine splitting and mixing amplitudes for ddμ ($J=1, \nu=1$) in meV ($K=1000$), including nuclear finite-size effects.

			amplitudes $\beta_{I,S}$	
$\mathcal{J}$	IS	$\varepsilon_{\mathcal{J},I,S}$	$\beta_{1,1/2}$	$\beta_{1,3/2}$
$\frac{1}{2}$	$1\,\frac{1}{2}$	−15.90	0.999 87	−0.016 06
	$1\,\frac{3}{2}$	7.64	0.016 06	0.999 87
$\frac{3}{2}$	$1\,\frac{1}{2}$	−16.13	0.999 94	−0.011 40
	$1\,\frac{3}{2}$	7.93	0.011 40	0.999 94
$\frac{5}{2}$	$1\,\frac{3}{2}$	8.22	0.000 00	1.000 00

TABLE XII. Total relativistic correction to ddμ binding energy in meV.

Contributions to relativistic shift	
Darwin correction	−0.89
Relativistic mass correction	0.46
Recoil	1.87
Total relativistic shift	1.44
Vacuum polarization (Uehling potential)	8.66
Nuclear finite-size correction to Coulomb potential	−1.54
Lowest hyperfine state	15.99
Total correction	24.55
Additional corrections	
Deuteron polarizability[a]	−0.1
Total correction to binding energy	24.5

[a]Value from Bakalov (Ref. 7).

For ddμ it is possible to compare the final results with experimentally determined binding energies. The experimental binding energy excluding hyperfine splitting is −1965.9(5) meV,[26] the calculated value in this work is −1966.4 meV.

ACKNOWLEDGMENTS

This work has been supported by the Division of Advanced Energy Projects of the U.S. Department of Energy, Grant No. DE-FG05-ER13447. The authors wish to thank Dr. Steve Alexander and Dr. Susan Haywood for many useful and instructive discussions.

APPENDIX A: FINITE-SIZE EFFECTS

According to Bakalov[24] the electromagnetic form factors can be expanded in terms of a set of generalized dipole functions

$$F_{ij}(q^2)=\sum_{s=1}^{n_{ij}} \frac{w_{ijs}}{(1+q^2/\Lambda_{ijs}^2)^{l_{ijs}}}\ , \tag{A1}$$

where i refers to the particle and j, $1\le j\le 2s_i+1$, labels the different form factors (charge, magnetic, etc.) of particle i. The parameters w_{ijs}, Λ_{ijs}, and l_{ijs} are fitted to experimental form factors obtained from elastic scattering experiments. In the relativistic three-body Hamiltonian used in this work three types of form factors appear, e.g., $g_{(1)}(r)$, $\hat{g}_{(2)}(r)$, and $\hat{g}_{(3)}(r)$. These functions are defined by[27]

TABLE XIII. Comparison of results for dtμ from different authors.

	Bakalov (Ref. 19)[a]	Korobov (Ref. 21)[a]	Myint (Ref. 20)[b]	This work[a]	This work[b]
Scalar terms[c]	30.0	30.7	28.5	30.8	28.3
Lowest hyperfine state	35.9	35.2		35.2	35.2
Total	65.9	65.9		66.0	63.5

[a]Results using form-factor data from Ref. 23.
[b]Results using form-factor data from Ref. 22.
[c]Does not include deuteron polarizability and molecular finite-size effect.

$$g_{(n)}(r)=1-r\int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{r}}\frac{4\pi}{k^2}G_{(n)}(k^2)\ ,\quad n=1,2,2',3 \tag{A2}$$

and similarly

$$\hat{g}_{(n)}(r)=\frac{g''_{(n)}(r)}{r}-4\pi[g_{(n)}(r)-1]\delta(\mathbf{r})\ . \tag{A3}$$

The functions $G_{(n)}(k^2)$ are defined as

$$\begin{aligned}
G_{(1)}&=F_{i1}F_{j1}\ ,\\
G_{(2)}&=\frac{Z_iF_{i1}-(\mu_i/s_i)F'_{i2}}{Z_i-(\mu_i/s_i)}F_{j1}\ ,\\
G_{(2')}&=F_{i1}\frac{Z_jF_{j1}-(\mu_j/s_j)F'_{j2}}{Z_j-(\mu_j/s_j)}\ ,\\
G_{(3)}&=F'_{i2}F'_{j2}\ ,
\end{aligned} \tag{A4}$$

where

$$F'_{i2}=\begin{cases}(Z_iF_{i1}+A_iF_{i2})/\mu_i, & s_i=\frac{1}{2}\\ F_{i2}, & s_i=1\end{cases} \tag{A5}$$

where $A_i=\mu_i-Z_i$. Because the muon is considered to be pointlike and the internuclear effects can be neglected (being several orders of magnitude smaller than the μ-nuclear effect), the functions $g_{(n)}(r)$ can be shown to have the form

$$g_{(n)}(r)=\sum_t W_{ijt}a_{l_t}(r,\Lambda_{ijt})\ , \tag{A6}$$

where the coefficients W_{ijt} can be found by combining Eqs. (A1), (A2), (A4), and (A5), and

$$\begin{aligned}
a_l(r,\Lambda)&=1-r\int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{r}}\left[1+\frac{k^2}{\Lambda^2}\right]^{-l}\frac{4\pi}{k^2}\\
&=e^{-\Lambda r}\sum_{k=0}^{l-1}c_k^l(\Lambda r)^k\ ,
\end{aligned} \tag{A7}$$

with $c_0^l=1$ and

$$c_k^l=\frac{2^k}{(k-1)!}\sum_{p=k}^{l-1}\frac{(2p-k-1)!}{4^p(p-k)!p!}\quad\text{for } k\geq 1\ . \tag{A8}$$

From this we can easily derive that

$$\begin{aligned}
\hat{a}_l(r,\Lambda)&=\frac{a_l''(r,\Lambda)}{r}\\
&=\Lambda^3e^{-\Lambda r}\sum_{k=0}^{l-2}\hat{c}_k^{\,l}(\Lambda r)^k\ ,
\end{aligned} \tag{A9}$$

with

$$\hat{c}_k^{\,l}=\frac{2^{k+3-2l}(2l-k-4)!}{k!(l-1)!(l-k-2)!}\ . \tag{A10}$$

To calculate the effect of the inclusion of these form factors into the Hamiltonian, one therefore has to evaluate integrals of the type [using the definition $\Omega_n(r)=r^ne^{-\Lambda r}$]

$$\begin{aligned}
A_{n+k,l,m}&=\tfrac{1}{2}\int_0^\infty r_1^k dr_1\int_0^\infty r_2^l dr_2\int_{|r_1-r_2|}^{r_1+r_2}r_{12}^m dr_{12}\Omega_n(r_1)e^{-(ar_1+br_2+cr_{12})}\\
&=\tfrac{1}{2}\int_0^\infty r_1^k dr_1\int_0^\infty r_2^l dr_2\int_{|r_1-r_2|}^{r_1+r_2}r_{12}^m dr_{12}r_1^n e^{-\Lambda r_1}e^{-(ar_1+br_2+cr_{12})}\ .
\end{aligned} \tag{A11}$$

For $k=l=m=0$ this reduces to

$$A_{n,0,0}=\tfrac{1}{2}\int_0^\infty dr_1\int_0^\infty dr_2\int_{|r_1-r_2|}^{r_1+r_2}dr_{12}r_1^n e^{-\Lambda r_1}e^{-(ar_1+br_2+cr_{12})}\ . \tag{A12}$$

This integral can easily be evaluated and gives

$$A_{n,0,0}=\frac{(-1)^n n!}{(b+c)(b-c)}\left[\frac{1}{(a+\Lambda+b)^n}-\frac{1}{(a+\Lambda+c)^n}\right]\ . \tag{A13}$$

Because $\Lambda\gg 1$ we can expand this expression in powers of $1/\Lambda$, giving

$$\begin{aligned}
A_{n,0,0}\approx\frac{1}{(b+c)}\frac{1}{\Lambda^{n+2}}\Bigg[&(n+1)!-\frac{(n+2)!}{2\Lambda}(2a+b+c)+\frac{(n+3)!}{6\Lambda^2}[3a^2+3a(b+c)+b^2+bc+c^2]\\
&-\frac{(n+4)!}{24\Lambda^3}[4a^3+6a^2(b+c)+4a(b^2+bc+c^2)+(b^3+b^2c+c^2b+c^3)]\Bigg]\ .
\end{aligned} \tag{A14}$$

For the evaluation of the nuclear finite-size effects for p states, we need the integrals $A_{n+3,1,1}$, $A_{n+1,3,1}$, and $A_{n+1,1,3}$. These can be obtained by repeated derivation of $A_{n,0,0}$, with respect to b and c and yields the following expressions [up to $O(1/\Lambda^{n+5})$]:

$$A_{n,1,1}\approx\frac{2}{\Lambda^{n+2}(b+c)^3}\left[(n+1)!-\frac{(n+2)!}{\Lambda}a+\frac{(n+3)!}{\Lambda^2}\left[\frac{a^2}{2}-\frac{bc}{6}\right]-\frac{(n+4)!}{\Lambda^3}\left[\frac{a(a^2-bc)}{6}\right]\right], \tag{A15}$$

$$A_{n,3,1}\approx\frac{2}{\Lambda^{n+2}(b+c)^5}\left[12(n+1)!-\frac{12(n+2)!}{\Lambda}a+\frac{(n+3)!}{\Lambda^2}[6a^2+c(c-b)]-\frac{(n+4)!}{\Lambda^3}a[2a^2+c(c-b)]\right], \tag{A16}$$

and

$$A_{n,1,3}\approx\frac{2}{\Lambda^{n+2}(b+c)^5}\left[12(n+1)!-\frac{12(n+2)!}{\Lambda}a+\frac{(n+3)!}{\Lambda^2}[6a^2+b(b-c)]+\frac{(n+4)!}{\Lambda^3}a[2a^2+b(b-c)]\right]. \tag{A17}$$

For the $J=1$ states of dtμ and ddμ the basis functions can be written as $|i\rangle=z_1|i,1\rangle\pm z_2|i,2\rangle$ (see Sec. II). We therefore have to calculate three types of integrals. Explicitly they are

$$\langle i,1|\Omega_n|j,1\rangle=\frac{16\pi^2}{3}A_{n+3,1,1}, \tag{A18}$$

$$\langle i,1|\Omega_n|j,2\rangle=\frac{8\pi^2}{3}(A_{n+3,1,1}+A_{n+1,3,1}-A_{n+1,1,3}), \tag{A19}$$

and

$$\langle i,2|\Omega_n|j,2\rangle=\frac{16\pi^2}{3}A_{n+1,3,1}. \tag{A20}$$

We can now use the explicit forms of c_k^l and $\hat{c}_k^l$ to obtain the relations

$$\sum_{k=0}^{l-1}c_k^l(k+n)!=\frac{\Gamma(n+1)\Gamma(l+(n+1)/2)}{\Gamma(1+(n+1)/2)\Gamma(l)} \tag{A21}$$

and

$$\sum_{k=0}^{l-2}\hat{c}_k^l(k+n)!=\frac{\Gamma(n)\Gamma(l-1+n/2)}{\Gamma(n/2)\Gamma(l)}. \tag{A22}$$

We can now evaluate the matrix elements of the two finite-size operators occurring in the relativistic Hamiltonian. For the nuclear finite-size correction to the Coulomb operator we find [up to $O(\Lambda^{-2})$ and ignoring the fact that we have to take linear combinations of operators], with $g=\sum_n c_n^l\Lambda^n\Omega_n$

$$\langle i,1|g(r_1)/r_1|j,1\rangle\approx\frac{8\pi^2}{3}\frac{3l(l+1)}{\Lambda^4}\frac{4}{(b+c)^3}, \tag{A23}$$

$$\langle i,1|g(r_1)/r_1|j,2\rangle\approx\frac{4\pi^2}{3}\frac{3l(l+1)}{\Lambda^4}\left[\frac{4}{(b+c)^3}+\frac{4[6a^2+c(c-b)]}{(b+c)^5}-\frac{4[6a^2+b(b-c)]}{(b+c)^5}\right], \tag{A24}$$

and

$$\langle i,2|g(r_1)/r_1|j,2\rangle\approx\frac{8\pi^2}{3}\frac{1}{\Lambda^2}\left[\frac{48l}{(b+c)^5}-\frac{4l(2l+1)!!}{(2l)!!\Lambda}\frac{a}{(b+c)^5}+\frac{12l(l+1)}{\Lambda^2}\frac{[6a^2+c(c-b)]}{(b+c)^5}\right]. \tag{A25}$$

The matrix elements of the nuclear finite-size corrections to the δ functions we find equivalently, with $\hat{g}=g''/r$

$$\langle i,1|\hat{g}(r_1)|j,1\rangle\approx\frac{8\pi^2}{3}\frac{6l}{\Lambda^2}\frac{4}{(b+c)^3}, \tag{A26}$$

$$\langle i,1|\hat{g}(r_1)|j,2\rangle\approx\frac{4\pi^2}{3}\frac{6l}{\Lambda}\left[\frac{4}{(b+c)^3}+\frac{4}{(b+c)^5}[6a^2+c(c-b)]-\frac{4}{(b+c)^5}[6a^2+b(b-c)]\right], \tag{A27}$$

and finally

$$\langle i,2|\hat{g}(r_1)|j,2\rangle\approx\frac{8\pi^2}{3}\left[\frac{48}{(b+c)^5}-\frac{2(2l-1)!!}{(2l-2)!!\Lambda}\frac{48a}{(b+c)^5}+\frac{6l}{\Lambda^2}\frac{4[6a^2+c(c-b)]}{(b+c)^5}\right], \tag{A28}$$

where a, b, and c are the appropriate combinations of exponential parameters. The expressions for $g(r_2)$ and $\hat{g}(r_2)$ are easily obtained by exchanging parameters a with b, and labels 1 with 2 in all expressions. The finite-size corrections for the internuclear terms are at least one order of magnitude smaller and can thus be neglected.

APPENDIX B: MATRIX ELEMENTS OF THE UEHLING POTENTIAL

The Uehling potential for particles of charges Z_1 and Z_2 and distance r is given by[13]

$$U_{\mathrm{VP}}(r)=\frac{2\alpha Z_1 Z_2}{3\pi}V_U(r)$$
$$=\frac{2\alpha Z_1 Z_2}{3\pi r}\int_1^\infty dx\frac{(x^2-1)^{1/2}(1+1/2x^2)e^{-2\gamma x r}}{x^2}\ . \tag{B1}$$

This leads to integrals of the type

$$I_{l,m,n}=\int\int dv_1 dv_2 V_U(r_{12})r_1^l r_2^m r_{12}^n e^{-(ar_1+br_2+cr_{12})}\ . \tag{B2}$$

In a basis of Slater geminals the integration over the volume elements can easily be performed for $l=m=n=-1$,

$$I_{-1,-1,-1}=\frac{16\pi^2}{(a+b)}\int_1^\infty\frac{dx[1+1/(2x^2)](x^2-1)^{1/2}}{x^2(a+c+2\gamma x)(b+c+2\gamma x)}$$
$$=\frac{16\pi^2}{(a+b)}\tilde{I}_{-1,-1,-1}\ . \tag{B3}$$

The last integral can be integrated to give

$$\tilde{I}_{-1,-1,-1}=\frac{-4}{(a+c+2\gamma)(b+c+2\gamma)}$$
$$\times[2G_{0,1,1}(p,q)+G_{1,1,1}(p,q)]\ , \tag{B4}$$

with $p=(a+c-2\gamma)/(a+c+2\gamma)$, $q=(b+c-2\gamma)/(b+c+2\gamma)$, and

$$G_{K,L,M}(p,q)=\int_\infty^1\frac{dt\,t^2(t^2-1)^{2K+L+M-1}}{(t^2+1)^{2K+2}(t^2-p)^L(t^2-q)^M}\ . \tag{B5}$$

The general expression can then be found by differentiation with respect to a, b, and c. This results in

$$I_{l,m,n}=\frac{-64\pi^2}{(a+b)}\sum_{i=0}^{l+1}\sum_{j=0}^{m+1}\sum_{k=0}^{n+1}\binom{l+1}{i}\binom{m+1}{j}\binom{n+1}{k}\frac{(i+j)!(l-i+k+1)!(m+n+2-k-j)!}{(a+b)^{i+j}(a+c+2\gamma)^{l-i+k+2}(b+c+2\gamma)^{m+n+3-k-j}}$$
$$\times[2G_{0,l+k+2,m+n+3-k}(p,q)+G_{1,l+k+2,m+n+3-k}(p,q)]\ . \tag{B6}$$

The integrals $G_{K,L,M}(p,q)$ can be evaluated analytically, but the expressions become numerically highly unstable for $p\approx q$ and are therefore calculated by numerical integration.

APPENDIX C: MATRIX ELEMENTS OF SPIN OPERATORS

In general, the relativistic operators are spin dependent. Averaging over space and spin variables, however, can be separated, for both the zeroth-order perturbative wave function and the relativistic Hamiltonian can always be factorized in a space-dependent part and a spin-dependent part. After the space integration has been performed an effective spin Hamiltonian is obtained containing only spin and angular momentum operators.[27,28] The matrix elements involving spin and angular momentum operators can be expressed using the Wigner-Eckart theorem. The spin functions for the three-particle system are considered to be coupled as follows. First the nuclear spins $\mathbf{s}_1$ and $\mathbf{s}_2$ are coupled to $\mathbf{I}$. Then $\mathbf{I}$ and $\mathbf{s}_3$ are coupled to the total spin $\mathbf{S}$. Finally the total spin is coupled to the orbital angular momentum $\mathbf{J}$ to give the total momentum $\mathcal{F}$. The total wave function can then be expressed as

$$|\mathcal{F}\mathcal{M}\rangle=|s_1 s_2;Is_3;SJ;\mathcal{F}\mathcal{M}\rangle\ . \tag{C1}$$

In the nonrelativistic case these states form a degenerate set. This degeneracy is lifted by the spin-dependent relativistic interactions. In first-order perturbation theory the stationary hyperfine states are eigenvectors of the effective spin Hamiltonian and can be found as linear combinations of the functions $|IS\mathcal{F}\rangle$ that have a definite value of I and S:

$$|\mathcal{F}N\rangle=\sum_{I,S}\beta_{IS}^{\mathcal{F}N}|IS\mathcal{F}\rangle\ , \tag{C2}$$

where N numbers different states with the same $\mathcal{F}$ with eigenvalues $\varepsilon_{\mathcal{F}IS}^N$, and $\beta_{IS}^{\mathcal{F}N}=\langle IS\mathcal{F}|\mathcal{F}N\rangle$. The latter have to be determined by diagonalizing the effective spin Hamiltonian.

The matrix element of any scalar operator with respect to these wave functions can then be written as

$$\langle s_1' s_2';I's_3';S'J';\mathcal{F}'\mathcal{M}'|\mathsf{R}^a\cdot\mathsf{S}^a|s_1 s_2;Is_3;SJ;\mathcal{F}\mathcal{M}\rangle=\delta_{\mathcal{F}'\mathcal{F}}\delta_{\mathcal{M}'\mathcal{M}}(-1)^{\mathcal{F}+S+J'}\begin{Bmatrix}S' & S & a\\ J & J' & \mathcal{F}\end{Bmatrix}\langle I'S'\|\mathsf{S}^a\|IS\rangle\langle J'\|\mathsf{R}^a\|J\rangle\ . \tag{C3}$$

Here $\mathsf{R}^a\cdot\mathsf{S}^a$ denotes the scalar product of two tensor operators and rank a, and $\langle I'S'\|\mathsf{S}^a\|IS\rangle$ and $\langle J'\|\mathsf{R}^a\|J\rangle$ and reduced matrix elements of the involved tensor operators.

The relativistic operators introduced in Sec. II involve only three different types of spin operators, i.e., scalar operator products

$$F_{ij}=\langle s_1' s_2';I's_3';S'\|\mathbf{s}_i\cdot\mathbf{s}_j\|s_1 s_2;Is_3;S\rangle\ , \tag{C4}$$

vector operators

$$S_i=\langle s_1's_2';I's_3';S'\|\mathbf{s}_i\|s_1s_2;Is_3;S\rangle\ , \tag{C5}$$

and tensor operators of rank 2

$$T_{ij}=\langle s_1's_2';I's_3';S'\|(\mathbf{s}_i\otimes\mathbf{s}_j)^{(2)}\|s_1s_2;Is_3;S\rangle\ . \tag{C6}$$

Using the notations

$$R_i=\langle s_i'\|\mathbf{s}_i\|s_i\rangle=\delta_{s_i',s_i}\sqrt{s_i(s_i+1)(2s_i+1)}\ , \tag{C7}$$

$$\Pi_{abc\ldots}=\sqrt{(2a+1)(2b+1)(2c+1)(\cdots)\cdots}\ , \tag{C8}$$

and

$$\sigma=s_1+s_2+s_3+S, \tag{C9}$$

we find for the scalar product operators

$$F_{23}=\delta_{S'S}(-1)^{\sigma+I+I'+1}\Pi_{II'S}R_2R_3\begin{Bmatrix}s_2&1&s_2\\I&s_1&I'\end{Bmatrix}\times\begin{Bmatrix}I'&1&I\\s_3&S&s_3\end{Bmatrix}, \tag{C10}$$

$$F_{13}=\delta_{S'S}(-1)^{\sigma+2I+1}\Pi_{II'S}R_1R_3\begin{Bmatrix}s_1&1&s_1\\I&s_2&I'\end{Bmatrix}\times\begin{Bmatrix}I'&1&I\\s_3&S&s_3\end{Bmatrix}, \tag{C11}$$

$$F_{12}=(-1)^{I+s_1+s_2}\Pi_SR_1R_2\begin{Bmatrix}S_1&1&S_1\\S_2&I&S_2\end{Bmatrix}, \tag{C12}$$

for the vector operators

$$S_1=(-1)^{\sigma+I'+I}\Pi_{II'SS'}R_1\begin{Bmatrix}s_1&1&s_1\\I&s_2&I'\end{Bmatrix}\begin{Bmatrix}I'&1&I\\S&s_3&S'\end{Bmatrix}, \tag{C13}$$

$$S_2=(-1)^{\sigma+2I'}\Pi_{II'SS'}R_2\begin{Bmatrix}s_2&1&s_2\\I&s_1&I'\end{Bmatrix}\begin{Bmatrix}I'&1&I\\S&s_3&S'\end{Bmatrix}, \tag{C14}$$

$$S_3=\delta_{I'I}(-1)^{s_3+I+S'+1}\Pi_{SS'}R_3\begin{Bmatrix}s_3&1&s_3\\S&I&S'\end{Bmatrix}, \tag{C15}$$

and for the tensor operators

$$T_{11}=(-1)^{I+I'+\sigma}\left[\frac{(2s_1-1)(2s_1+3)}{6}\right]^{1/2}\Pi_{II'SS'R_1}\begin{Bmatrix}s_1&2&s_1\\I'&s_2&I\end{Bmatrix}\begin{Bmatrix}S'&2&S\\I&s_3&I'\end{Bmatrix}, \tag{C16}$$

$$T_{22}=(-1)^{2I'+\sigma}\left[\frac{(2s_2-1)(2s_2+3)}{6}\right]^{1/2}\Pi_{II'SS'R_2}\begin{Bmatrix}s_2&2&s_2\\I'&s_1&I\end{Bmatrix}\begin{Bmatrix}S'&2&S\\I&s_3&I'\end{Bmatrix}, \tag{C17}$$

$$T_{33}=\delta_{II'}(-1)^{I+S'+s_3}\left[\frac{(2s_3-1)(2s_3+3)}{6}\right]^{1/2}\Pi_{SS'R_3}\begin{Bmatrix}s_3&2&s_3\\S'&I&S\end{Bmatrix}, \tag{C18}$$

$$T_{23}=(-1)^{I'+s_1+s_2+1}\Pi_{II'SS'2}R_2R_3\begin{Bmatrix}s_2&1&s_2\\I&s_1&I'\end{Bmatrix}\begin{Bmatrix}I&s_3&S\\1&1&2\\I'&s_3&S'\end{Bmatrix}, \tag{C19}$$

$$T_{13}=(-1)^{I+s_1+s_2+1}\Pi_{II'SS'2}R_1R_3\begin{Bmatrix}s_1&1&s_1\\I&s_2&I'\end{Bmatrix}\begin{Bmatrix}I&s_3&S\\1&1&2\\I'&s_3&S'\end{Bmatrix}, \tag{C20}$$

$$T_{12}=(-1)^{I'+S+s_3}\Pi_{II'SS'2}R_1R_2\begin{Bmatrix}I&2&I'\\S'&s_3&S\end{Bmatrix}\begin{Bmatrix}s_1&s_2&I\\1&1&2\\s_1&s_2&I'\end{Bmatrix}. \tag{C21}$$

For muonic molecules both s_1 and s_2 are less than or equal to 1 and $s_3=\frac{1}{2}$. This can be used to reduce the $9j$ symbols occurring in the last three expressions to more easily calculated combinations of $6j$ symbols.

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