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Addition/Correction

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Correction to "Calculation of the Positron Annihilation Rate in PsH with the Positronic Extension of the Explicitly Correlated Nuclear-Electronic Orbital Method"

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Since publication of this article, we identified errors in the computer code used to generate some of the results. The corrected results are given in the tables below. These corrections do not alter the conclusions of the paper, and the agreement between the NEO-XCHF annihilation rate and the ECG and SVM benchmark values in Table 3 is improved.

Table 1. Values for Parameters (a.u.) Defining the Gaussian-Type Geminal Functions Optimized with the 6s/6s Basis Set

N_{gem}	b_1	γ_1	b_2	γ_2	b_3	γ_3	b_4	γ_4
1	2.2740	0.1910						
2	2.3968	0.8466	2.3027	0.1136				
3	2.0740	0.0810	2.6730	0.4370	1.7130	2.9300		
4	1.8212	0.0637	2.6878	0.2948	1.9883	1.3385	1.1246	8.8371

Table 2. Total Energies E and Annihilation Rates λ for PsH with Different Basis Sets

	E (a.u.)		λ (ns^{-1})	
method[a]	6s/6s	9s/6s[b]	6s/6s	9s/6s[b]
NEO-HF	−0.664337	−0.665640	0.3190	0.3201
NEO-XCHF 1G	−0.723303	−0.724497	1.0905	1.0914
NEO-XCHF 2G	−0.735139	−0.736326	1.7498	1.7508
NEO-XCHF 3G	−0.737081	−0.738270	2.0892	2.0903
NEO-XCHF 4G	−0.737423	−0.738613	2.2616	2.2626

[a]NEO-XCHF nG is with $N_{gem} = n$, and the basis sets are defined by the number of electronic/positronic basis functions. [b]The 9s/9s results are the same as the 9s/6s results for the energies to within 10^{-5} a.u. and the rates to within 10^{-4} ns^{-1}.

Table 3. Total Energies E and Annihilation Rates λ for PsH

method	E (a.u.)	λ (ns^{-1})
NEO-HF[a]	−0.665640	0.3201[d]
NEO-FCI[b]	−0.758965	0.8993
NEO-XCHF[c]	−0.738613	2.2626
ECG (ref 1)	−0.789197	2.471406
SVM (ref 2)	−0.789197	2.47178

[a]NEO-HF result with the 9s/6s basis set. [b]NEO-FCI result with the 6s3p1d basis set.[3] [c]NEO-XCHF result with four geminal functions and the 9s/6s basis set. The positron is bound to H^- by 6.9 eV at this level of theory. [d]Note that this NEO-HF value was incorrectly reported in ref 4.

■ ACKNOWLEDGMENTS

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■ REFERENCES

(1) Bubin, S.; Adamowicz, L. *Phys. Rev. A* **2006**, *74*, 052502.
(2) Mitroy, J. *Phys. Rev. A* **2006**, *73*, 054502.
(3) Adamson, P. E.; Duan, X. F.; Burggraf, L. W.; Pak, M. V.; Swalina, C.; Hammes-Schiffer, S. *J. Phys. Chem. A* **2008**, *112*, 1346.
(4) Swalina, C.; Pak, M. V.; Hammes-Schiffer, S. *J. Chem. Phys.* **2012**, *136*, 164105.

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