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Erratum: “Theoretical transition probabilities for the OH Meinel system” [J. Chem. Phys. 126, 114314 (2007)]

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We recently discovered errors in our code for calculating the OH Meinel transitions which was used in calculations for two recent works.^{1,2}

The weak $F_1 \leftarrow F_2$ and $F_2 \leftarrow F_1$ transitions of OH in the $X^2\Pi(v, J, p)$ states were neglected, yielding a difference in total lifetimes of OH $X^2\Pi(v=1, J=3/2, F_1, p)$ states of about 2.5% or 1.4 ms. Furthermore, we found a phase difference in the basis sets used to implement the rotational Hamiltonian of Eq. (2) and the lambda-doubling Hamiltonian of Eqs. (8)–(10). Finally, we found an inconsistency in the implementation of the spin-orbit Hamiltonian. The equations in the paper are consistent.

In the new calculations we also replace the $r_e = 1.8342a_0$ value by a more recent value³ of $r_e = 1.8324a_0$.

The new calculations affect the numbers in Tables IV and V, which are reproduced here in Tables I and II. Our electric dipole moment function yields slightly higher values for the expectation values of the dipole moment than

experimentally observed. Therefore, in Table II, we also include a lifetime based on our dipole moment function scaled with a factor of 0.9966. This is the average ratio between the experimentally observed ($v=0, 1, 2$) dipole moment and our *ab initio* values.

Finally, we make available a new EPAPS document⁴ based on the corrected calculations. The line strengths are computed using the partition function $Q(T=296)=80.362$ from the HITRAN database. The changes reported here do not significantly alter our conclusions.

TABLE I. Computed and experimental vibrationally averaged dipole moments of OH in ea_0 .

v	Exp. ^a	Present	L89 ^b	WRR ^c
0	0.65120(4)	0.6527	0.6570	0.6457
1	0.65411(6)	0.6561	0.6598	0.6481
2	0.6550(4)	0.6582	0.6611	0.6490
3		0.6585	0.6605	0.6479
4		0.6567	0.6578	0.6446
5		0.6522	0.6524	0.6386
6		0.6444	0.6437	0.6291
7		0.6324	0.6311	0.6157
8		0.6153	0.6136	0.5974
9		0.5919	0.5901	0.5731

^aPeterson *et al.* (Ref. 5). Converted from Debye using 1 Db = 0.39343031369 ea_0 .

^bLanghoff *et al.* (Ref. 6).

^cWerner *et al.* (Ref. 7).

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TABLE II. Lifetime (in ms) of the OH($v=1, J=3/2, F_1, p$) states, computed using various dipole moment functions and methods.

Exp.	$e(-)$	$f(+)$	Error bars	
Direct ^a		59.0	± 2 ms	
HITRAN ^b	56.6113	56.6244	± 10 –20%	
	$H_{so}(r)$		$H_{ \Omega , \Omega' }^{so}$	
Calc.	$e(-)$	$f(+)$	$e(-)$	$f(+)$
μ_{sc} ^c	57.2246	57.2253	57.2235	57.2242
present ^d	56.8364	56.8371	56.8354	56.8360
nosc ^e	56.8835	56.8842	56.8824	56.8831
ω_H ^f	56.8359	56.8366	56.8272	56.8278
N90 ^g	55.7004	55.7011	55.6989	55.6996
L89 ^h	57.7759	57.7766	57.7742	57.7749
WRR ⁱ	71.6343	71.6352	71.6319	71.6328
L86 ^j	81.3144	81.3154	81.3104	81.3114
M71 ^k	85.6512	85.6522	85.6480	85.6490

^aExperiment by van de Meerakker *et al.* (Ref. 1).

^bComputed from the HITRAN 2004 (Ref. 8) database.

^cScaled potential and scaled dipole moment.

^dThis work, using the scaled potential.

^eThis work, using the *ab initio* potential.

^fThis work, using HITRAN transition frequencies.

^gFitted dipole moment function by Nelson (Ref. 9).

^h*Ab initio* dipole moment function by Langhoff *et al.* (Ref. 6).

ⁱ*Ab initio* dipole moment function by Werner *et al.* (Ref. 7).

^j*Ab initio* dipole moment function by Langhoff *et al.* (Ref. 10).

^kFitted dipole moment function by Murphy (Ref. 11).

- ¹S. Y. T. van de Meerakker, N. Vanhaecke, M. P. J. van der Loo, G. C. Groenenboom, and G. Meijer, *Phys. Rev. Lett.* **95**, 013003 (2005).
- ²M. P. J. van der Loo and G. C. Groenenboom, *J. Chem. Phys.* **126**, 114314 (2007).
- ³P. C. Cosby, private communication, the r_e value was determined by constructing an RKR-potential from the constants in Table II of the paper.
- ⁴See EPAPS Document No. E-JCPSA6-128-022814 for computed potential energy curve and properties. For more information on EPAPS, see <http://www.aip.org/pubservs/epaps.html>.
- ⁵K. I. Peterson, G. T. Fraser, and W. Klemperer, *Can. J. Phys.* **62**, 1502 (1984).
- ⁶S. R. Langhoff, C. W. Bauschlicher, and P. R. Taylor, *J. Chem. Phys.* **91**, 5953 (1989).
- ⁷H.-J. Werner, P. Rosmus, and E.-A. Reinsch, *J. Chem. Phys.* **79**, 905 (1983).
- ⁸L. Rothman, D. Jacquemart, A. Barbe, D. C. Benner, M. Birk, L. R. Brown, M. Carleer, C. Chackerian, Jr., K. Chance, L. H. Coudert, V. Dana, V. M. Devi, J.-M. Flaud, R. R. Gamache, A. Goldman, J.-M. Hartmann, K. W. Jucks, A. G. Maki, J.-Y. Mandin, S. T. Massie, J. Orphal, A. Perrin, C. P. Rinsland, M. A. H. Smith, J. Tennyson, R. N. Tolchenov, R. A. Toth, J. Vander Auwera, P. Varanasi, and G. Wagner, *J. Quant. Spectrosc. Radiat. Transf.* **96**, 139 (2005).
- ⁹D. D. Nelson, Jr., A. Schiffman, D. J. Nesbitt, J. J. Orlando, and J. B. Burkholder, *J. Chem. Phys.* **93**, 7003 (1990).
- ¹⁰S. R. Langhoff, H.-J. Werner, and P. Rosmus, *J. Mol. Spectrosc.* **118**, 507 (1986).
- ¹¹R. E. Murphy, *J. Chem. Phys.* **54**, 4852 (1971).