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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 $r_e = 1.8342 a_0$ value by a more recent value[3] of $r_e = 1.8324 a_0$.

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 document[4] 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

[a] Peterson *et al.* (Ref. 5). Converted from Debye using 1 Db $=0.39343031369\ ea_0$.
[b] Langhoff *et al.* (Ref. 6).
[c] Werner *et al.* (Ref. 7).

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%	
	$H_{\rm so}(r)$		$H^{\rm so}_{\vert\Omega\vert,\vert\Omega'\vert}$	
Calc.	$e(-)$	$f(+)$	$e(-)$	$f(+)$
$\mu_{\rm sc}$[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

[a] Experiment by van de Meerakker *et al.* (Ref. 1).
[b] Computed from the HITRAN 2004 (Ref. 8) database.
[c] Scaled potential and scaled dipole moment.
[d] This work, using the scaled potential.
[e] This work, using the *ab initio* potential.
[f] This work, using HITRAN transition frequencies.
[g] Fitted 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).
[k] Fitted dipole moment function by Murphy (Ref. 11).

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[4] See 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.

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