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Erratum

Erratum to: ''Coupled cluster calculations of Verdet constants'' [Chem. Phys. Lett. 281 (1997) 445] [1]

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A small error has been detected in the multiplicative factor employed to obtain the Verdet constant in au from the computed response functions. The results of our investigation given in the tables should be multiplied by 1.005695. All conclusions remain valid, except for H_2, where our FCI/d-aug-ccpV5Z results are now in excellent agreement with the explicitly correlated results of Ref. [9]. The correct results for hydrogen are given in Table 1.

Two misprints have also been found:

1. Eq. (3): the constant C is

$$C = \frac{1}{6c}\left(\frac{2\pi N}{4\pi\varepsilon_0}\right)\left(\frac{e}{2m_e}\right).$$

2. 1 au of $V(\omega)$ (rad $ea_0\hbar$) $= 2.763816 \times 10^2$ min G^{-1} cm^{-1}.

Table 1
FCI Verdet constants of H_2 (au $\times 10^7$)

Basis set	ω (au)			
	0.11391	0.08284	0.06509	0.05360
cc-pVQZ	0.22640	0.11607	0.07070	0.04761
aug-cc-pVQZ	0.45643	0.22998	0.13912	0.09335
d-aug-cc-pVQZ	0.45679	0.23002	0.13911	0.09334
t-aug-cc-pVQZ	0.45665	0.22995	0.13907	0.09331
cc-pV5Z	0.28236	0.14421	0.08773	0.05903
aug-cc-pV5Z	0.45597	0.22965	0.13887	0.09319
d-aug-cc-pV5Z	0.45562	0.22944	0.13876	0.09310
Ref. [9] [a]	0.45556	0.22946	0.13877	0.09312
Ref. [9] [b]	0.50527	0.25361	0.15316	0.10270
Exp. [10]	0.501	0.251	0.150	0.103

[a] Equilibrium geometry. [b] Ro-vibrationally and thermally averaged values.

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