

Erratum: “Hyperfine interactions and internal rotation in methanol” [J. Chem. Phys. 145, 244301 (2016)]

Boy Lankhaar, Gerrit C. Groenenboom, and Ad van der Avoird

Citation: *The Journal of Chemical Physics* **148**, 149901 (2018); doi: 10.1063/1.5030801

View online: <https://doi.org/10.1063/1.5030801>

View Table of Contents: <http://aip.scitation.org/toc/jcp/148/14>

Published by the [American Institute of Physics](#)



Erratum: “Hyperfine interactions and internal rotation in methanol” [J. Chem. Phys. **145**, 244301 (2016)]

 Boy Lankhaar,^{1,2,a)} Gerrit C. Groenenboom,¹ and Ad van der Avoird¹
¹Theoretical Chemistry, Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

²Department of Earth and Space Sciences, Chalmers University of Technology, Onsala Space Observatory, 439 92 Onsala, Sweden

(Received 26 March 2018; accepted 3 April 2018; published online 10 April 2018)

<https://doi.org/10.1063/1.5030801>

Table II in Ref. 1, giving the Fourier expansion coefficients of the spin-torsion tensors, was reported erroneously. The correct values are given in Table I. We note that the generated hyperfine spectra, or any other results in Ref. 1, are not affected by this change, as this error only concerns Table II in Ref. 1.

TABLE I. Coefficients a_n^{nuc} in the Fourier expansion describing the γ dependence of the nuclear contribution to the spin-torsion coupling vectors $\mathbf{d}_K(\gamma)$ calculated from the nuclear coordinates. The electronic contribution a_0^{el} , assumed to be γ -independent, is obtained from a fit to measured hyperfine spectra; see text. The components of \mathbf{d}_K are defined with respect to the principal axes a , b , and c . Their γ dependence is expanded in functions $\cos n\gamma$ terms or $\sin n\gamma$ for + and – symmetry, respectively. The superscripts CH₃ and OH refer to the CH₃ protons ($K = 1, 2, 3$) and OH proton ($K = 4$), respectively. Results are given only for the CH₃ proton with $K = 1$, and the values for $K = 2, 3$ correspond to a change of γ by 120° and 240°, respectively. All spin-torsion coupling expansion coefficients a_n and the coefficients a_n^{T} of the Thomas precession corrections \mathbf{q}_K/I_γ are given in kHz.

	Symmetry	a_0^{nuc}	a_1^{nuc}	a_2^{nuc}	a_3^{nuc}	a_6^{nuc}	a_0^{el}	a_1^{el}	a_2^{el}	a_3^{el}	a_6^{el}	$a_0^{\text{T}}(\approx a_6^{\text{T}})$
$d_a^{\text{CH}_3}$	+	79.996	1.304	0	0	0	–66.410	–5.518	–0.075	0.050	0	$-1.31 \cdot 10^{-8}$
$d_b^{\text{CH}_3}$	+	4.435	–23.527	0	0	0	–10.163	19.098	0.485	–0.132	0	$-2.91 \cdot 10^{-6}$
$d_c^{\text{CH}_3}$	–	0	23.563	0	0	0	0	–18.880	–0.508	0.129	0	0
d_a^{OH}	+	11.658	0	0	–0.136	–0.001	–0.462	0	0	–0.245	–0.001	0
d_b^{OH}	+	21.480	0	0	–0.190	–0.001	–53.987	0	0	0.141	0.001	0
d_c^{OH}	–	0	0	0	0.245	0.001	0	0	0	–0.246	–0.002	0

¹B. Lankhaar, G. Groenenboom, and A. van der Avoird, “Hyperfine interactions and internal rotation in methanol,” *J. Chem. Phys.* **145**(24), 244301 (2016).

a) Current address: Department of Earth, Space and Environment, Chalmers University of Technology, Onsala Space Observatory, 439 92 Onsala, Sweden.