The Journal of Chemical Physics

ERRATUM | FEBRUARY 06 2024

Erratum: "Breaking covalent bonds in the context of the many-body expansion (MBE). I. The purported 'first row anomaly' in XH_n (X = C, Si, Ge, Sn; n = 1–4)" [J. Chem. Phys. 156, 244303 (2022)]

Demeter Tzeli ; Sotiris S. Xantheas

J. Chem. Phys. 160, 059901 (2024)
https://doi.org/10.1063/5.0196893

The Journal of Chemical Physics ERRATUM pubs.aip.org/aip/jcp

Erratum: "Breaking covalent bonds in the context of the many-body expansion (MBE). I. The purported 'first row anomaly' in XH_n (X = C, Si, Ge, Sn; n = 1–4)" [J. Chem. Phys. 156, 244303 (2022)]

Cite as: J. Chem. Phys. 160, 059901 (2024); doi: 10.1063/5.0196893
Submitted: 10 January 2024 • Accepted: 15 January 2024 •
Published Online: 6 February 2024

Demeter Tzeli[1,2] and Sotiris S. Xantheas[3,4,5,a)]

AFFILIATIONS

[1] Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens 15784, Greece
[2] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece
[3] Advanced Computing, Mathematics and Data Division, Pacific Northwest National Laboratory, 902 Battelle Boulevard, P.O. Box 999, MSIN J7-10, Richland, Washington 99352, USA
[4] Department of Chemistry, University of Washington, Seattle, Washington 98195, USA
[5] Computational and Theoretical Chemistry Institute (CTCI), Pacific Northwest National Laboratory, Richland, Washington 99352, USA

Note: This paper is part of the JCP Special Topic on Nature of the Chemical Bond.

[a)] **Author to whom correspondence should be addressed:** sotiris.xantheas@pnnl.gov and xantheas@uw.edu

https://doi.org/10.1063/5.0196893

TABLE V. Bond distances R_{XH} (Å) and angles φ_{HXH} (degrees) of the calculated states of XH_n (X = C, Si, Ge, Sn; n = 1–4) at the RCCSD(T) level of theory.

		CH_n			SiH_n	GeH_n	SnH_n
		AVDZ	AVTZ	AVQZ	AVQZ	AVQZ	AVQZ
$XH(\chi^2\Pi)$	R_{XH}	1.1400	1.1219	1.1203	1.5242	1.6028	1.7901
$XH(A^4\Sigma^-)$	R_{XH}	1.1066	1.0908	1.0894	1.4969	1.5694	1.7550
$XH(\alpha^2\Delta)$	R_{XH}	1.1229	1.1069	1.1056			
$XH_2(^3B_1)$	R_{XH}	1.0943	1.0791	1.0775	1.4815	1.5449	1.7281
	φ_{HXH}	133.06	133.56	133.61	118.38	119.41	118.61
$XH_2(^1A_1)$	R_{XH}	1.1271	1.1107	1.1088	1.5184	1.5963	1.7841
	φ_{HXH}	101.14	101.88	102.01	92.28	91.65	91.20
$XH_3(X^2A_1)$	R_{XH}	1.0932	1.0795	1.0780	1.4810	1.5443	1.7289
	φ_{HXH}	120.00	120.00	120.00	107.59	107.68	109.21
$XH_4(X^1A_1)$	R_{XH}	1.1027	1.0899	1.0883	1.4803	1.5414	1.7289
	φ_{HXH}	109.47	109.47	109.47	109.49	109.47	109.21

We have noted typographical errors in Table V of the published article.[1] Specifically, the values of the angles $\varphi_{H\chi H}$ for the XH_2 species in both the ($^3B_1$) and ($^1A_1$) states were incorrectly reported as half of the correct values. The values of the same angles for the XH_3 and XH_4 species were reported correctly. The table with the corrected values is below.

ACKNOWLEDGMENTS

S.S.X. was supported from the Center for Scalable Predictive methods for Excitations and Correlated phenomena (SPEC), which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division as part of the Computational Chemical Sciences (CCS) program under FWP 70942 at Pacific Northwest National Laboratory (PNNL), a multiprogram national laboratory operated for DOE by Battelle. This research also used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

REFERENCE

[1] D. Tzeli and S. S. Xantheas, "Breaking covalent bonds in the contest of the many-body expansion (MBE). I. The purported 'first row anomaly' in XH_n (X = C, Si, Ge, Sn; n = 1–4)," J. Chem. Phys. **156**, 244303 (2022).