

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  

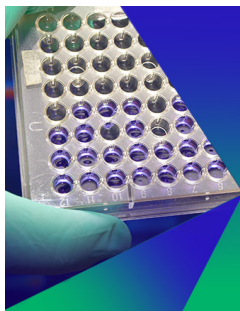


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**Note:** This paper is part of the JCP Special Topic on Nature of the Chemical Bond.

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**TABLE V.** Bond distances  $R_{XH}$  (Å) and angles  $\varphi_{HXH}$  (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	1.7550
	$XH(\alpha^2\Delta)$	$R_{XH}$	1.1229	1.1069	1.1056		
$XH_2(^3B_1)$	$R_{XH}$	1.0943	1.0791	1.0775	1.4815	1.5449	1.7281
	$\varphi_{HXH}$	133.06	133.56	133.61	118.38	119.41	118.61
	$R_{XH}$	1.1271	1.1107	1.1088	1.5184	1.5963	1.7841
$XH_2(^1A_1)$	$\varphi_{HXH}$	101.14	101.88	102.01	92.28	91.65	91.20
	$R_{XH}$	1.0932	1.0795	1.0780	1.4810	1.5443	1.7289
$XH_3(X^2A_1)$	$\varphi_{HXH}$	120.00	120.00	120.00	107.59	107.68	109.21
	$R_{XH}$	1.1027	1.0899	1.0883	1.4803	1.5414	1.7289
$XH_4(X^1A_1)$	$\varphi_{HXH}$	109.47	109.47	109.47	109.49	109.47	109.21

We have noted typographical errors in [Table V](#) of the published article.<sup>1</sup> Specifically, the values of the angles  $\varphi_{\text{HXH}}$  for the  $\text{XH}_2$  species in both the ( $^3\text{B}_1$ ) and ( $^1\text{A}_1$ ) states were incorrectly reported as half of the correct values. The values of the same angles for the  $\text{XH}_3$  and  $\text{XH}_4$  species were reported correctly. The table with the corrected values is below.

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## REFERENCE

<sup>1</sup>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  $\text{XH}_n$  ( $X = \text{C}, \text{Si}, \text{Ge}, \text{Sn}$ ;  $n = 1-4$ )," *J. Chem. Phys.* **156**, 244303 (2022).