ERRATUM

Erratum to: Theoretical reference values for the AE6 and BH6 test sets from explicitly correlated coupled-cluster theory

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In the original publication of the article, some barrier heights for the reactions $H + OH \rightarrow O + H_2$ and $H + H_2S \rightarrow H_2 + SH$ and one atomization energy of the values reported are incorrect due to a small error which occured during addition of individual contributions. The correct atomization energy for SiO for FC-CCSD(T)/cc-pVQZ-F12 $+ \delta_{HE} + \delta_{C/CV}$ is 801.7 kJ/mol. The affected levels of theory for the barrier heights are FC-CCSD(T)/cc-pV(Q+d)Z $+ \delta_{HE} + \delta_{C/CV}$, FC-CCSD(T)/cc-pV(5+d)Z $+ \delta_{HE} + \delta_{C/CV}$, FC-CCSD(T)/cc-pV(6+d)Z $+ \delta_{HE} + \delta_{C/CV}$, and FC-CCSD(T)/CBS $+ \delta_{HE} + \delta_{C/CV}$. The correct values are given in Table 1.

After rectifying the errors mentioned, the values calculated on the FC-CCSD(T)(F12)/cc-pVQZ-F12 $+ \delta_{HE} + \delta_{C/CV}$ level of theory agree even better with the values on the FC-CCSD(T)/CBS $+ \delta_{HE} + \delta_{C/CV}$ level of theory.

None of these corrections affect the other tables nor the conclusion in the original article. The authors would like to thank Konstantinos Vogiatzis for making them aware of these errors.

Table 1 (revised part of Table 2) Barrier heights for the reactions of the BH6 test set in kJ/mol

	$H + OH \rightarrow O + H_2$		$H + H_2S \rightarrow H_2 + SH$	
	$E_{\text{fwd}}^{\neq}$	$E_{\text{rev}}^{\neq}$	$E_{\text{fwd}}^{\neq}$	$E_{\text{rev}}^{\neq}$
FC-CCSD(T)/cc-pV(Q+d)Z $+ \delta_{HE} + \delta_{C/CV}$	44.4	58.0	16.6	73.6
FC-CCSD(T)/cc-pV(5+d)Z $+ \delta_{HE} + \delta_{C/CV}$	44.9	55.7	16.2	72.2
FC-CCSD(T)/cc-pV(6+d)Z $+ \delta_{HE} + \delta_{C/CV}$	45.0	55.0	16.0	71.7
FC-CCSD(T)/CBS $+ \delta_{HE} + \delta_{C/CV}$	45.1	53.9	15.8	71.0

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