Thermochemical Kinetics of Hydrogen-Atom Transfers Between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen

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Table 3 in the paper is not correct. The corrected table is:

Table 3 Expectation values of Total Spin, $\langle \hat{S}^2 \rangle$, for Selected Species Using Different

Methods	<i>a</i> .
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Species	HF	HF//MP2	HF//BMC-CCSD	MPW1K	M06-L
CH ₃	0.76	0.76	0.76	0.76	0.76
ССН	1.12	1.02	1.17	0.80	0.78
H–H–H	0.79	0.79	0.79	0.76	0.76
СНЗ-Н-СНЗ	0.79	0.79	0.79	0.76	0.769
НСС-Н-ССН	1.22	1.11	1.41	0.80	0.78
НСС-Н-Н	1.07	1.02	1.18	0.80	0.78

^{*a*} In this table, the basis set is MG3S.