Erratum: "Fewest-switches with time uncertainty: A modified trajectory surface-hopping algorithm with better accuracy for classically forbidden electronic transitions" [J. Chem. Phys. 116, 5424 (2002)]

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The FSTU calculations in the paper[1] were carried out using the reflect-and-hop-back treatment for frustrated hops, which is denoted[2] (−,−), rather than (as incorrectly stated) by ignoring frustrated hops, which is denoted (+,+). This affects only those frustrated hops that could not be fixed by nonlocal hopping. The TFS calculations were carried out as reported, i.e., using the (+,+) method. Presented here are the corrected tables. Table I includes additional rows that show the TFS (−,−) and FSTU (−,−) results for comparison. The (+,+) method does better for the final vibrational and rotational quantum numbers, and the (−,−) method does better for F_R, which agrees with our previous[2] observation.

Table II also contains an error: The F_R and P_N column labels are interchanged.

The overall conclusions of the paper are not changed.

TABLE I. Mean unsigned relative errors (MUREs) for the TFS and FSTU methods averaged over 12 test cases.

Method	P_R	$\langle v' \rangle$	$\langle j' \rangle$	P_Q	$\langle v'' \rangle$	$\langle j'' \rangle$	P_N	F_R	Prob.[a]	Mom.[b]	All[c]
TFS (+,+)[d]	1.36	0.12	0.14	0.29	0.23	0.67	0.32	0.93	0.73	0.29	0.51
TFS (−,−)[d]	0.97	0.20	0.15	0.39	0.40	0.85	0.37	0.63	0.59	0.40	0.50
FSTU (+,+)	1.25	0.14	0.15	0.21	0.27	0.79	0.19	1.12	0.69	0.34	0.51
FSTU (−,−)[e]	0.73	0.17	0.14	0.19	0.38	0.91	0.16	0.67	0.44	0.40	0.42

[a]Average MURE for the probabilities P_R, P_Q, F_R, and P_N.
[b]Average MURE for the moments $\langle v' \rangle$, $\langle j' \rangle$, $\langle v'' \rangle$, and $\langle j'' \rangle$.
[c]Average MURE for all eight observables.
[d]The MUREs for the TFS method were computed from the data in Ref. 2.
[e]Previously published in Ref. 1 and incorrectly denoted FSTU (+,+).

TABLE II. Unsigned relative errors (UREs) for the TFS and FSTU methods for the 12 test cases.

		P_N		F_R	
I. C.[a]	U_{12}^{max}/eV	TFS (+,+)	FSTU (+,+)	TFS (+,+)	FSTU (+,+)
(1.10, 0)	0.20	0.75	0.38	0.64	0.71
	0.10	0.18	0.06	0.48	0.57
	0.03	0.49	0.15	0.31	0.37
	0.01	0.43	0.33	0.14	0.07
(1.10, 6)	0.20	0.15	0.01	0.47	0.54
	0.10	0.41	0.26	0.61	0.66
	0.03	0.05	0.10	0.39	0.31
	0.01	0.05	0.11	0.41	0.51
(1.02, 0)	0.20	0.91	0.66	0.32	0.50
	0.10	0.11	0.09	3.23	3.58
	0.03	0.21	0.05	1.93	2.30
	0.01	0.16	0.07	2.25	3.26
Mean[b]		0.32	0.19	0.93	1.12

[a]Initial conditions are specified in Sec. II of Ref. 1.
[b]Average of 12 cases.

[1] A. W. Jasper, S. N. Stechmann, and D. G. Truhlar, J. Chem. Phys. **116**, 5424 (2002).

[2] A. W. Jasper, M. D. Hack, and D. G. Truhlar, J. Chem. Phys. **115**, 1804 (2001).

