Benchmark Quantum Mechanical Calculations of Vibrationally Resolved Cross Sections and Rate Constants on *ab initio* Potential Energy Surfaces for the F+HD Reaction: Comparisons with Experiments

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Supporting Information

Table S1. Comparison of the calculated rate constants (in cm^3 $molecule^{-1}$ s^{-1} $\times$ 10^{-13}) for the HF formation on the LWAL, CSZ, FXZ and SW PESs as a function of temperature.

T(K)	LWAL	CSZ	FXZ		SW		
	This Work	This Work	This Work	Ref.[1]	This Work	Ref.[2]	Ref.[3]
10	.630	.837	.470		2.51		
20	.849	.944	.524		2.36		
40	3.68	3.64	2.19		4.99		
60	8.52	8.54	5.91		11.7		
80	13.0	13.2	9.83		19.8		
100	17.4	17.7	13.7	13.7	27.9	28.7	27.1
120	22.2	22.6	17.9	17.9	35.8	36.4	35.4
140	27.8	28.3	22.8	22.8	44.0	44.3	43.9
160	34.5	35.1	28.7	28.7	52.7	52.6	52.9
180	42.1	42.9	35.5	35.5	61.8	61.4	62.2
200	50.6	51.5	43.1	43.1	71.4	70.7	72.0
220	59.7	60.7	51.5	51.4	81.5	80.3	82.2
240	69.2	70.4	60.4	60.2	91.8	90.1	92.7
260	79.1	80.5	69.8	69.4	102	100	103
280	89.2	90.8	79.4	78.8	113	110	114
300	99.5	101	89.4	88.3	124	120	125
320	110	112			134		
340	120	122			145		
350	125	127			150		152

Table S2. Comparison of the calculated rate constants (in cm^3 $molecule^{-1}$ s^{-1} $\times$ 10^{-13}) for the DF formation on the LWAL, CSZ, FXZ and SW PESs as a function of temperature.

T(K)	LWAL	CSZ	FXZ		SW		
	This Work	This Work	This Work	Ref.[1]	This Work	Ref.[2]	Ref.[3]
10	.067	.099	.065		.469		
20	.077	.099	.066		.423		
40	.155	.177	.122		.600		
60	.391	.418	.292		1.12		
80	1.00	1.03	.735		2.28		
100	2.24	2.28	1.67	1.67	4.39	4.3	4.36
120	4.31	4.36	3.29	3.29	7.63	7.6	7.61
140	7.30	7.36	5.71	5.71	12.0	11.9	11.9
160	11.2	11.3	8.99	8.99	17.4	17.3	17.4
180	16.0	16.1	13.1	13.0	23.7	23.6	23.7
200	21.5	21.6	17.9	17.8	30.8	30.6	30.7
220	27.7	27.8	23.4	23.3	38.5	38.2	38.3
240	34.4	34.5	29.4	29.2	46.6	46.3	46.3
260	41.5	41.6	35.9	35.5	55.0	54.6	54.6
280	48.9	49.0	42.7	42.1	63.5	63.1	63.1
300	56.5	56.5	49.8	48.9	72.2	71.7	71.7
320	64.1	64.2			80.6		
340	71.8	71.9			89.4		
350	75.7	75.7			93.6		93.4

References

[1] De Fazio, D.; Lucas, J. M.; Aquilanti , V.; Cavalli, S. Exploring the accuracy level of new potential energy surfaces for the F + HD reactions: from exact quantum rate constants to the state-to-state reaction dynamics. *Phys. Chem. Chem. Phys.* **2011**, *13*, 8571-8582.

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[3] Zhang, D.H.; Lee, S.-Y.; Baer, M. Quantum mechanical integral cross sections and rate constants for the F+HD reactions. *J. Chem. Phys.* **2000**, *112*, 9802-9809.