

Supplementary Material:

Quantum dynamics and kinetics of the F+H₂ and F+D₂ reactions at low and ultra-low temperatures

1 SUPPLEMENTARY TABLES AND FIGURES

The input data for the F+H₂ and F+D₂ quantum scattering calculations on the SW potential energy surface and PES II are given in Table S1 and Table S2.

Table S1. Input parameters used in the production run of the F+H₂ reaction.

E/meV	J	Kmax	j	emax	rmax	mtr	prod	dE/meV
<i>SW PES</i>								
96-145	20	6	18	2.3	10	100	100	0.5
46-95	17	5	18	2.3	15	150	100	0.5
22-42	13	3	18	3.0	15	150	100	0.2
2.2-21.9	11	3	18	2.5	20	200	99	0.2
1.2-2.2	7	3	18	2.3	20	235	100	1.0(-2)
0.2-1.2	5	3	18	2.3	25	300	104	1.0(-2)
<i>risuk</i>								
1.4(-1)-1.6(-1)	4	3	20	3.3	25	700	18	4.0(-4)
1.1(-2)-1.4(-1)	4	2	16	3.0	30	300	128	1.0(-3)
1.0(-3)-1.1(-2)	2	1	16	2.5	28	320	97	1.0(-4)
0.6(-4)-1.0(-3)	1	1	16	2.8	35	400	100	1.0(-5)
0.8(-5)-0.6(-4)	0	0	16	2.8	35	400	50	1.0(-6)
<i>PES II</i>								
96-145	21	6	18	2.3	15	150	100	0.05
46-95	19	5	18	2.3	20	200	100	0.05
22-42	13	3	24	3.0	18	180	100	0.02
2.1-21.9	11	2	24	3.0	25	250	100	0.02
1.1-2.1	7	2	16	2.5	30	300	100	1.0(-2)
0.3-1.1	6	1	16	2.5	40	400	84	1.0(-2)
<i>risuk</i>								
	6						37	1.0(-3/-4)
6.9(-2)-2.7(-1)	4	1	16	2.5	50	500	100	2.0(-3)
1.1(-2)-5.3(-2)	3	2	80	3.8	80	1000	86	0.5(-3)
1.0(-3)-1.1(-2)	2	1	18	3.0	100	1000	98	1.0(-4)
1.0(-4)-1.0(-3)	2	1	16	2.5	140	1400	94	1.0(-5)
1.0(-5)-1.0(-4)	1	0	16	2.5	180	1800	91	1.0(-6)
0.4(-6)-1.0(-5)	0	0	16	2.5	220	2200	100	1.0(-7)

For explanation of input parameters see Skouteris et al. (2000); De Fazio (2014); De Fazio et al. (2016).

Table S2. Input parameters used in the production run for the F+D₂ reaction.

E/meV	J	K _{max}	j	e _{max}	r _{max}	mtr	prod	dE/meV
<i>SW PES</i>								
39.9-72.1	19	4	25	3.0	15	150	130	0.25
22.4-39.6	15	3	28	3.0	20	275	70	0.25
2.3-22.2	14	2	20	2.5	20	350	200	0.01
0.22-2.19	11	2	20	2.5	35	500	198	1.0(-2)
2.0(-2)-2.2(-1)	6	1	20	2.5	70	1030	198	1.0(-3)
2.2(-3)-2.2(-2)	2	2	34	2.8	100	1325	198	1.0(-4)
2.2(-4)-2.2(-3)	2	1	25	3.0	130	1750	198	1.0(-5)
2.2(-5)-2.2(-4)	1	1	22	3.0	150	2025	198	1.0(-6)
2.0(-6)-2.2(-5)	0	0	22	3.0	180	2435	200	1.0(-7)
<i>PES II</i>								
39.9-72.1	19	4	25	3.0	15	150	130	0.25
22.4-39.6	15	3	28	3.0	20	275	70	0.25
2.3-22.2	14	2	20	2.5	20	350	200	0.01
0.22-2.19	11	2	20	2.5	35	500	198	1.0(-2)
2.0(-2)-2.2(-1)	6	1	20	2.5	70	1030	198	1.0(-3)
2.2(-3)-2.2(-2)	2	2	34	2.8	100	1325	198	1.0(-4)
2.2(-4)-2.2(-3)	2	1	25	3.0	130	1750	198	1.0(-5)
2.2(-5)-2.2(-4)	1	1	22	3.0	150	2025	198	1.0(-6)
2.0(-6)-2.2(-5)	0	0	22	3.0	180	2435	200	1.0(-7)

For explanation of input parameters see Skouteris et al. (2000); De Fazio (2014); De Fazio et al. (2016).

REFERENCES

- Skouteris, D., Castillo, J., and Manolopoulos, D. (2000). Abc: a quantum reactive scattering program. *Computer Physics Communications* 133, 128–135
- De Fazio, D. (2014). The H+HeH⁺ → He + H₂⁺ reaction from the ultra-cold regime to the three-body breakup: exact quantum mechanical integral cross sections and rate constants. *Physical Chemistry Chemical Physics* 16, 11662–11672
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